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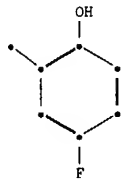
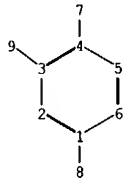
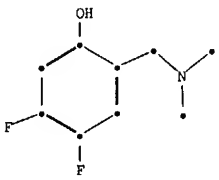


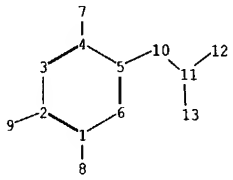


chain nodes :
    7 8 9
ring nodes :
    1 2 3 4 5 6
chain bonds :
    1-8 3-9 4-7
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
    4-7
exact bonds :
    1-8 3-9
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
    containing 1 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS

C:\Program Files\Stnexp\Queries\758-4.str

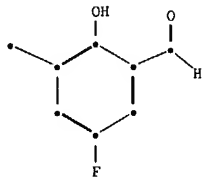


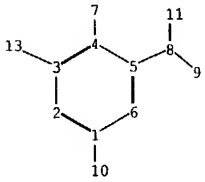


chain nodes :
7 8 9 10 11 12 13
ring nodes :
1 2 3 4 5 6
chain bonds :
1-8 2-9 4-7 5-10 10-11 11-12 11-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-7 10-11 11-12 11-13
exact bonds :
1-8 2-9 5-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS

C:\Program Files\Stnexp\Queries\758-2.str

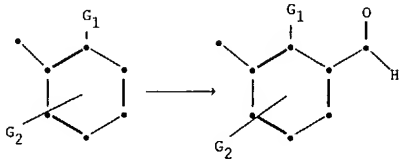


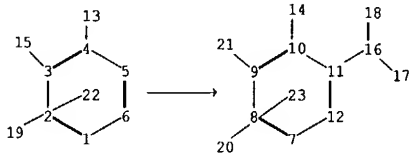


chain nodes :
7 8 9 10 11 13
ring nodes :
1 2 3 4 5 6
chain bonds :
1-10 3-13 4-7 5-8 8-9 8-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-7 8-11
exact bonds :
1-10 3-13 5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:CLASS

C:\Program Files\Stnexp\Queries\758.str



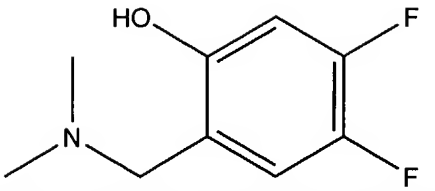


chain nodes :
13 14 15 16 17 18 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
3-15 4-13 9-21 10-14 11-16 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
4-13 10-14 16-18
exact bonds :
3-15 9-21 11-16 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

G1:H,OH

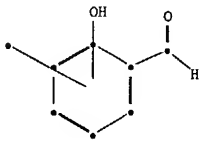
G2:F,CF3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1



4,5-difluoro-2hydroxy-N,N-dimethylbenzylamine

C:\Program Files\Stnexp\Queries\758-8.str



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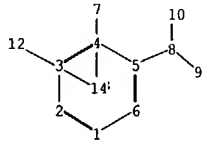

15

chain nodes :
7 8 9 10 12 15
ring nodes :
1 2 3 4 5 6
chain bonds :
5-8 8-10 8-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
8-10
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS

```
=> d his

     (FILE 'HOME' ENTERED AT 12:16:49 ON 30 JUL 2004)

     FILE 'REGISTRY' ENTERED AT 12:17:01 ON 30 JUL 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3             STRUCTURE UPLOADED
L4           1 S L3
L5             SCREEN 1839
L6             STRUCTURE UPLOADED
L7             QUE L6 NOT L5
L8           1 S L7
L9             SCREEN 1839
L10            STRUCTURE UPLOADED
L11            QUE L10 NOT L9
L12          3 S L11
L13         39 S L11 SSS FUL

     FILE 'CAPLUS' ENTERED AT 12:26:30 ON 30 JUL 2004
L14         79 S L13
L15        ANALYZE L14 1- RN HIT :      38 TERMS

     FILE 'REGISTRY' ENTERED AT 12:27:12 ON 30 JUL 2004
L16          1 S 210039-65-9/RN
L17         38 S L13 NOT L16

     FILE 'CAPLUS' ENTERED AT 12:27:36 ON 30 JUL 2004
L18         69 S L17

     FILE 'REGISTRY' ENTERED AT 12:28:44 ON 30 JUL 2004
L19          2 S 57477-83-5/RN 58914-34-4/RN OR 58107-25-8/RN OR 116314-64-8/R
L20          4 S 57477-83-5/RN OR 58914-34-4/RN OR 58107-25-8/RN OR 116314-64-
L21         34 S L17 NOT L20

     FILE 'CAPLUS' ENTERED AT 12:30:07 ON 30 JUL 2004
L22         42 S L21

=> d l11
L11 HAS NO ANSWERS
L9             SCR 1839
L10            STR
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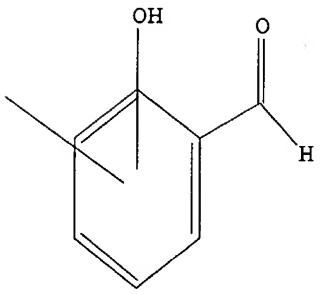


F

Structure attributes must be viewed using STN Express query preparation.
L11 QUE L10 NOT L9

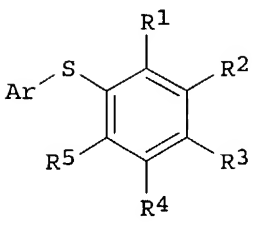
=> d ibib abs hitstr 1-42

L22 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:493573 CAPLUS
DOCUMENT NUMBER: 141:54069
TITLE: Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Gunawardana, Indrani W.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S. Pat. Appl. Publ., 133 pp., Cont. of U.S. Ser. No. 695,040.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

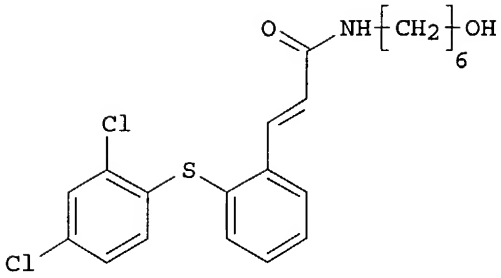
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004116518	A1	20040617	US 2003-725212	20031201

PRIORITY APPLN. INFO.:
US 1998-114097P P 19981229
US 1999-474517 B2 19991229
US 2000-541795 A2 20000331
US 2000-695040 A1 20001024

GI



I

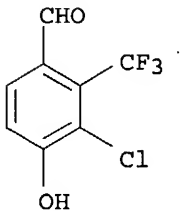


II

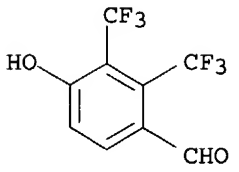
AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases and cerebral vasospasm. Examples include syntheses for 445 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp. The pharmaceutical composition comprising the compound I is claimed.

IT **280753-11-9P**, 3-Chloro-4-hydroxy-2-(trifluoromethyl)benzaldehyde
280753-16-4P, 4-Hydroxy-2,3-bis(trifluoromethyl)benzaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280753-11-9 CAPLUS
CN Benzaldehyde, 3-chloro-4-hydroxy-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



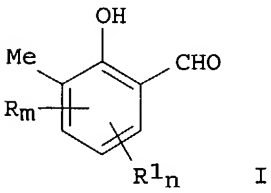
RN 280753-16-4 CAPLUS
CN Benzaldehyde, 4-hydroxy-2,3-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



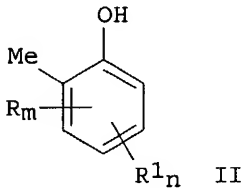
L22 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:485810 CAPLUS
DOCUMENT NUMBER: 141:38432
TITLE: Preparation of fluorine containing 2-hydroxy-3-methylbenzaldehydes
INVENTOR(S): Peilstoecker, Karen; Marhold, Albrecht
PATENT ASSIGNEE(S): Bayer Chemicals AG, Germany
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1428814	A1	20040616	EP 2003-26982	20031126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10257357	A1	20040624	DE 2002-10257357	20021209
US 2004133043	A1	20040708	US 2003-718758	20031121
JP 2004189741	A2	20040708	JP 2003-409405	20031208

PRIORITY APPLN. INFO.: DE 2002-10257357 A 20021209
GI



I

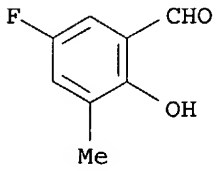


II

AB Title compds. [I; R1 = C1-12 alkyl, Cl, Br, ABDE, AE; A = C1-8 alkyl; B = O, S, NR2; R2 = H, C1-8 alkyl; D = carbonyl; E = C1-8 alkyl, C1-8 alkoxy, NH(C1-8 alkyl), N(C1-8 alkyl)2, cyclic amino group; n = 0-3m; R = F, C1-12 fluoroalkyl, O(C1-12 fluoroalkyl), S(C1-12 fluoroalkyl); m = 1-3], were prepd by reacting II (R, R1, m, and n as above) in the presence of urotropine and an acid or in the presence of formaldehyde and a secondary amine. Thus, 2-methyl-4-(trifluoromethoxy)phenol in CF3CO2H was dropwise treated with hexamethylenetetramine followed by heating at 100° for 16 h. After cooling, the reaction mixture was dropwise treated with 50% H2SO4 and then with H2O followed by stirring for 3 h at room temperature to give 34% 2-hydroxy-3-methyl-5-(trifluoromethoxy)benzaldehyde. The title compds. are especially useful for manufacturing agrochems. and drugs especially for treatment of cardiovascular diseases (no data).

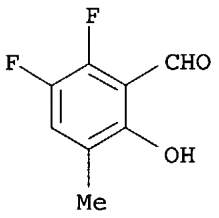
IT **704884-74-2P 704884-75-3P 704884-77-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

(Preparation)
(preparation of fluorine containing (hydroxy)(methyl)benzaldehydes)
RN 704884-74-2 CAPLUS
CN Benzaldehyde, 5-fluoro-2-hydroxy-3-methyl- (9CI) (CA INDEX NAME)

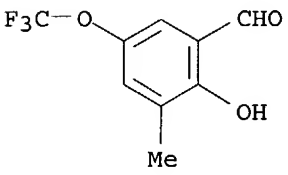


RN 704884-75-3 CAPLUS
CN Benzaldehyde, 2,3-difluoro-6-hydroxy-5-methyl- (9CI) (CA INDEX NAME)

Applicants

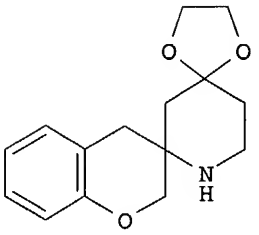


RN 704884-77-5 CAPLUS
CN Benzaldehyde, 2-hydroxy-3-methyl-5-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:58902 CAPLUS
DOCUMENT NUMBER: 140:181308
TITLE: A new efficient synthesis of spirocyclic benzopyrans
AUTHOR(S): Pave, Gregoire; Chalard, Pierre; Viaud-massuard, Marie-claude; Troin, Yves; Guillaumet, Gerald
CORPORATE SOURCE: Institut de Chimie Organique et Analytique, UMR CNRS 6005, Universite d'Orleans, Orleans, 45067/2, Fr.
SOURCE: Synthesis (2004), (1), 121-127
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

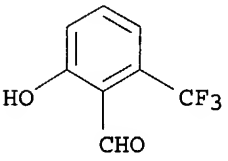


I

AB Starting from a protected β-amino ketone and several 3-chromanones, spirocyclic benzopyran derivs., e.g., I, were obtained via a Mannich type condensation.

IT **58914-35-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chromanones as precursors for spirocyclicbenzopyrans via condensation of salicylaldehydes with acrylonitrile followed by nitrile hydrolysis with subsequent Curtius reaction with diphenylphosphoryl azide followed by hydrolysis)

RN 58914-35-5 CAPLUS
CN Benzaldehyde, 2-hydroxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:991306 CAPLUS
DOCUMENT NUMBER: 140:41904
TITLE: Preparation of novel trifluoromethylepinephrine compounds as local analgesics and vasoconstrictors
INVENTOR(S): Ammann, Jeffrey R.
PATENT ASSIGNEE(S): U.S. Army Medical Research and Materiel Command, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103609	A2	20031218	WO 2003-US5976	20030228
WO 2003103609	A3	20040408		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,

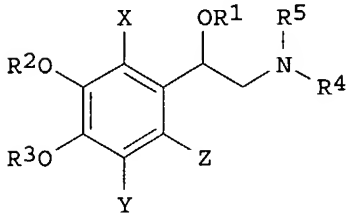
NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004015015 A1 20040122 US 2003-376311 20030303

PRIORITY APPLN. INFO.: US 2002-361510P P 20020304

OTHER SOURCE(S): MARPAT 140:41904

GI



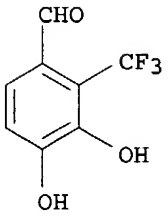
I

AB Disclosed herein are trifluoromethylepinephrine compds. having the following structural formula (I) (wherein R1-R5 are each independently selected from the group consisting of H, alkyl, alkoxyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, acyl, thioacyl, sulfonyl mercapto, alkylthio, carboxy, amino, alkylamino dialkylamino, carbamoyl, arylthio, and heteroarylthio; wherein X, Y, and Z are each independently selected from the group consisting of H or trifluoromethyl with the proviso that at least one of which is trifluoromethyl). Also disclosed are pharmaceutical compns. comprising the trifluoromethylepinephrine compds. and methods of making and using thereof. Novel trifluoroepinephrine intermediates are also disclosed. These compds. I are useful as analgesics, in particular local analgesics, and for treating a disease or a disorder associated with vasodilation or for inducing localized vasoconstriction.

IT **634924-69-9**, 3,4-Dihydroxy-2-trifluoromethylbenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel fluoromethylepinephrine compds. as analgesics or for treating disease or disorder associated with vasodilation)

RN 634924-69-9 CAPLUS

CN Benzaldehyde, 3,4-dihydroxy-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:698016 CAPLUS

DOCUMENT NUMBER: 140:217334

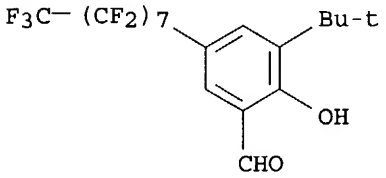
TITLE: Fluorous biphasic oxidation of sulfides catalyzed by (salen)manganese(III) complexes

AUTHOR(S): Cavazzini, Marco; Pozzi, Gianluca; Quici, Silvio; Shepperson, Ian

CORPORATE SOURCE: CNR-Istituto di Scienze e Tecnologie Molecolari, Milan, 20133, Italy

SOURCE: Journal of Molecular Catalysis A: Chemical (2003), 204-205, 433-441
CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Quadridentate Schiff base ligands derived from 1,2-diamines and fluorous derivs. of salicylaldehyde were prepared and their manganese(III) complexes were tested as catalysts in the selective oxidation of alkyl aryl sulfides with PhIO. Complexes bearing two fluorinated ponytails were soluble in standard organic solvents and were used under classical homogeneous conditions, whereas heavily fluorinated complexes could be used in an MeCN/perfluorooctane biphasic system. In both cases, sulfoxides were obtained as the main products, together with variable amts. of sulfones (≤10%), depending on the nature of the substrate and the catalyst. When reactions were carried out under fluorous biphasic conditions, the selectivity for sulfoxides was improved and the catalyst could be easily recovered by simple phase separation and reused up to four times. Despite their good chemoselectivity, catalytic efficiency and recyclability, chiral fluorous (salen)manganese(III) complexes showed low enantioselectivities in preliminary expts. run under fluorous biphasic conditions.
IT **417715-80-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorous biphasic oxidation of sulfides catalyzed by (salen)manganese(III) complexes)
RN 417715-80-1 CAPLUS
CN Benzaldehyde, 3-(1,1-dimethylethyl)-5-(heptadecafluorooctyl)-2-hydroxy- (9CI) (CA INDEX NAME)

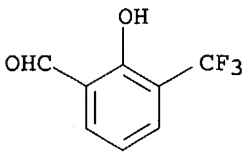


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:67246 CAPLUS
DOCUMENT NUMBER: 138:411019
TITLE: The synthesis and use in asymmetric epoxidation of metal salen complexes derived from enantiopure trans-cyclopentane- and cyclobutane-1,2-diamine
AUTHOR(S): Daly, Adrian M.; Gilheany, Declan G.
CORPORATE SOURCE: Conway Institute of Biomolecular and Biomedical Sciences, Centre for Synthesis and Chemical Biology, Chemistry Department, University College Dublin, Dublin, 4, Ire.
SOURCE: Tetrahedron: Asymmetry (2003), 14(1), 127-137
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:411019
AB A complete synthesis of enantiopure trans-cyclopentane-1,2-diamine and trans-cyclobutane-1,2-diamine is described. These diamines have been used as components of novel chiral salen ligands whose chromium and manganese complexes were then evaluated as oxygen transfer agents in the asym. epoxidn. of alkenes.
IT **336628-67-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chromium and manganese salen complexes derived from enantiopure trans-cyclopentanediamine and cyclobutanediamine and their catalytic performance for asym. epoxidn. of methylstyrene)

RN 336628-67-2 CAPLUS
CN Benzaldehyde, 2-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



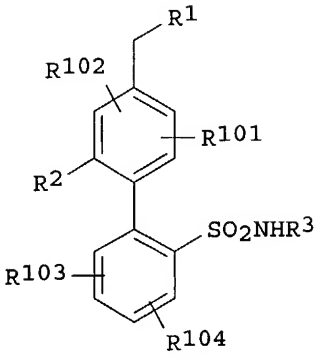
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:755214 CAPLUS
DOCUMENT NUMBER: 137:263024
TITLE: Preparation of N-isoxazolyl biphenylsulfonamides and related compounds as dual angiotensin II and endothelin receptor antagonists.
INVENTOR(S): Murugesan, Natesan; Tellew, John E.; Macor, Jhon E.; Gu, Zhengxiang
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: U.S. Pat. Appl. Publ., 206 pp., Cont.-in-part of U.S. Ser. No. 643,640, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002143024	A1	20021003	US 2000-737201	20001214
US 6638937	B2	20031028		
US 2004106833	A1	20040603	US 2003-673100	20030926
US 2004127515	A1	20040701	US 2003-672572	20030926

PRIORITY APPLN. INFO.:
US 1998-91847P P 19980706
US 1999-345392 B2 19990701
US 1999-464037 B2 19991215
US 2000-481197 B2 20000111
US 2000-513779 A2 20000225
US 2000-604322 A2 20000626
US 2000-643640 B2 20000822
US 2000-737201 A3 20001214

OTHER SOURCE(S): MARPAT 137:263024
GI



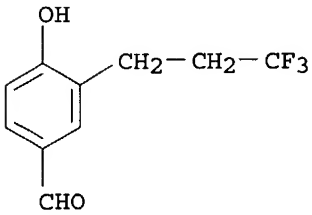
I

AB Title compds. (I; R1 = specified oxoimidazolyl, pyridoimidazolyl, pyridylamino, pyridyloxy, triazolyl, quinolinyloxy, etc.; R2 = H, halo, CHO, (halo)alkyl, cycloalkylalkyl, alkenyl, alkynyl, alkoxyalkyl, alkoxy, cyano, OH, NO2, etc.; R3 = heteroaryl; R101-R104 = H, halo, CHO, alkyl, haloalkyl, cycloalkylalkyl, alkenyl, alkynyl, alkoxyalkyl, haloalkoxyalkyl, alkoxy, alkoxyalkoxy, cyano, OH, hydroxyalkyl, NO2, etc; with provisos) were prepared as dual angiotensin II and endothelin receptor antagonists for treatment of hypertension and other diseases (no data). Thus, 4-BrC6H4CH2OH was coupled with [2-[[(4,5-dimethyl-3-isoxazolyl)[(2-methoxyethoxy)methyl]amino]sulfonyl]phenyl]boronic acid to give N-(4,5-dimethyl-3-isoxazolyl)-4'-(hydroxymethyl)-N-[(2-methoxyethoxy)methyl][1,1'-biphenyl]-2-sulfonamide (66%). This was brominated to give the 4'-bromomethyl derivative (90%), reacted with 2-butyl-1,3-diazaspiro[4.4]non-1-en-4-one hydrochloride, and deprotected (49% for two steps) to give 4'-[(2-butyl-4-oxo-1,3-diazaspiro[4.4]non-1-en-3-yl)methyl]-N-(4,5-dimethyl-3-isoxazolyl)-[1,1'-biphenyl]-2-sulfonamide.

IT **254745-93-2P**, Benzaldehyde, 4-hydroxy-3-(3,3,3-trifluoropropyl)-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-isoxazolyl biphenylsulfonamides and related compds. as dual angiotensin II and endothelin receptor antagonists)

RN 254745-93-2 CAPLUS

CN Benzaldehyde, 4-hydroxy-3-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 8 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:603826 CAPLUS

DOCUMENT NUMBER: 138:287905

TITLE: Synthesis of 6-[18F]fluoro-L-DOPA through nucleophilic 18F-fluoridation of carbonyl-activated aromatic amino acid, derivatives

AUTHOR(S): Tierling, Thomas

CORPORATE SOURCE: Inst. fuer Nuclearchemie, Germany

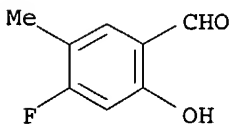
SOURCE: Berichte des Forschungszentrums Juelich (2002), Juel-3952, i-vi, 1-111

CODEN: FJBEE5; ISSN: 0366-0885
DOCUMENT TYPE: Report
LANGUAGE: German
OTHER SOURCE(S): CASREACT 138:287905

AB 6-[18F]Fluoro-L-3,4-dihydroxyphenylalanine (6-[18F]fluoro-L-DOPA), an analog of L-DOPA, is an established radiotracer for diagnostic PET-studies of the integrity and function of the nigrostriatal dopaminergic system. The use of this important compound in clin. centers is mainly limited by the lack of a nucleophilic radiofluorination method of preparation using the advantage of large scale production of [18F]fluoride. In this work a new convenient nucleophilic labeling method using [18F]fluoride was developed. With regard to the synthesis of 6-[18F]fluoro-L-DOPA via nucleophilic 18F-fluorination of carbonyl-activated aromatic amino acid derivs., several O-protected 4-fluoro-2-hydroxy-5-methyl-benzaldehydes were prepared as model compds. in order to evaluate the concept of synthesis. The 2-benzyloxy-4-[18F]fluoro-5-methyl-benzaldehyde was prepared via 18F-for-19F substitution with a radiochem. yield of 85 ± 5% and via 18F-for-N(CH3)3 substitution on (5-benzyloxy-4-formyl-2-methyl-phenyl)-trimethylammoniumtriflate with a radiochem. yield of 92 ± 5%. Thereof the synthesis of n.c.a. 2-benzyloxy-4-[18F]fluoro-5-methyl-phenol was achieved by Baeyer-Villiger oxidation with m-chloroperbenzoic acid with an overall radiochem. yield of 54 ± 5% within 40 min. An appropriate precursor for the synthesis of 6-[18F]fluoro-L-DOPA was synthesized by electrophilic alkylation of the lithiated bis-lactim ether (R)-2,5-dihydro-3,6-dimethoxy-2-isopropylpyrazine with 4-benzyloxy-2-fluoro-benzylbromide. The corresponding 5-(4-benzyloxy-2-fluoro-benzyl)-(2R,5S)-2,5-dihydro-3,6-dimethoxy-2-isopropylpyrazine, obtained with a diastereomeric excess of 84%, was formylated in the aromatic 5-position with dichloromethyl Me ether in the presence of a sixfold excess of tin(IV)chloride. The nucleophilic 18F-fluorination of 5-(4-benzyloxy-2-fluoro-5-formyl-benzyl)-(2R,5S)-2,5-dihydro-3,6-dimethoxy-2-isopropylpyrazine was performed in DMF at 130°C in the presence of the common Kryptofix 222/potassium carbonate system for 3 min. The radiochem. yield of the isotopic exchange was about 30 ± 5%. Baeyer-Villiger oxidation of 5-(4-benzyloxy-2-[18F]fluoro-5-formyl-benzyl)-(2R,5S)-2,5-dihydro-3,6-dimethoxy-2-isopropylpyrazine to the corresponding formate with m-chloroperbenzoic acid and subsequent hydrolysis and deprotection under strong acidic conditions led to the formation of c.a. 6-[18F]fluoro-DOPA with an enantiomeric excess of the L-isomer of about 70%. The overall radiochem. yield of 6-[18F]fluoro-L-DOPA was 14 to 18% within 70 min. According to the amount of 11 μmol precursor the carrier content is lower by a factor of about 10 in comparison to the electrophilic 18F-fluorination methods commonly used. Furthermore, use can be made of the fivefold higher production of [18F]fluoride compared to [18F]F2. However, the racemic mixture of 6-[18F]fluoro-L-DOPA still requires a chiral HPLC separation

IT **504414-06-6P**, 4-Fluoro-2-hydroxy-5-methylbenzaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 6-18F-L-3,4-dihydroxyphenylalanine through nucleophilic 18F-fluoridation of carbonyl-activated aromatic amino acid derivs.)

RN 504414-06-6 CAPLUS
CN Benzaldehyde, 4-fluoro-2-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



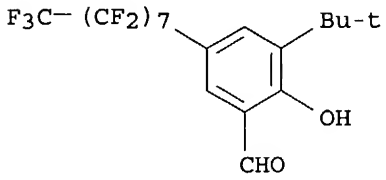
REFERENCE COUNT: 176 THERE ARE 176 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:11738 CAPLUS
DOCUMENT NUMBER: 136:355110
TITLE: Asymmetric epoxidation of alkenes in fluorinated media, catalyzed by second-generation fluorous chiral (salen)manganese complexes
AUTHOR(S): Cavazzini, Marco; Manfredi, Amedea; Montanari, Fernando; Quici, Silvio; Pozzi, Gianluca
CORPORATE SOURCE: Centro CNR Sintesi e Stereochimica di Speciali Sistemi Organici, Milan, 20133, Italy
SOURCE: European Journal of Organic Chemistry (2001), (24), 4639-4649
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:355110

AB The synthesis of sterically hindered chiral (salen)manganese complexes bearing perfluoroalkyl ponytails and their use in asym. epoxidn. reactions are described. For better understanding of the relative influences of steric and electronic effects on the enantioselectivity of the fluorous catalysts, the epoxidn. of 1,2-dihydronaphthalene and benzosuberene was first studied under homogeneous conditions. It was shown that the presence of sterically demanding tert-Bu groups and, to a lesser degree, the displacement of the electron-withdrawing perfluoroalkyl substituents from the ligand core provide ees higher than those attainable with first generation fluorous chiral (salen)manganese complexes featuring perfluoroalkyl substituents in the key positions (3,3' and 5,5') in the ligand. Second generation catalysts were successfully employed in the fluorous biphase epoxidn. of alkenes with PhIO as the oxidant and pyridine N-oxide as an additive. Epoxide yields (68-98%) and ees (50-92%) were similar to those obtained with the same oxidizing system and standard (salen)manganese complexes under homogeneous conditions. When the reaction was complete, the fluorous layer in which the catalyst was immobilized was easily recoverable by simple phase separation at room temperature and could be used up to three times before significant decline in yield and enantioselectivity was observed

IT **417715-80-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. epoxidn. of alkenes in fluorinated media, catalyzed by second-generation fluorous chiral (salen)manganese complexes)
RN 417715-80-1 CAPLUS
CN Benzaldehyde, 3-(1,1-dimethylethyl)-5-(heptadecafluorooctyl)-2-hydroxy- (9CI) (CA INDEX NAME)



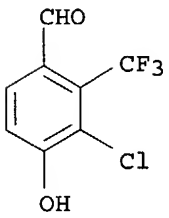
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

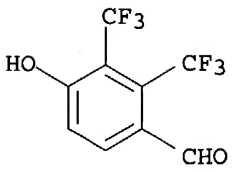
ACCESSION NUMBER: 2001:758465 CAPLUS
DOCUMENT NUMBER: 136:47984
TITLE: Discovery of Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 4. Structure-Activity Relationship of Substituents on the Benzene Ring of the Cinnamide
AUTHOR(S): Winn, Martin; Reilly, Edward B.; Liu, Gang; Huth, Jeffrey R.; Jae, Hwan-Soo; Freeman, Jennifer; Pei, Zhonghua; Xin, Zhili; Lynch, John; Kester, Jeff; von Geldern, Thomas W.; Leitza, Sandra; DeVries, Peter; Dickinson, Robert; Mussatto, Donna; Okasinski, Gregory F.
CORPORATE SOURCE: Metabolic Disease Research Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4393-4403
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have shown that p-arylthio cinnamides can inhibit the interaction of LFA-1 and ICAM-1, which is involved in cell adhesion and the inflammatory process. We now show that 2,3-disubstitution on the aryl portion of the cinnamide results in enhanced activity over mono substitution on the ring. The best 2,3-substituents were chlorine and trifluoromethyl groups. Compds. 39 and 40 which contain two CF3 groups have IC50 values of 0.5 and 0.1 nM, resp., in inhibiting JY8 cells expressing LFA-1 on their surface, from adhering to ICAM-1. The structure-activity relation (SAR) was examined using an NMR based model of the LFA-1 I domain/compound 31 complex. One of our compds. (38) was able to reduce cell migration in two different in vivo expts.

IT **280753-11-9P 280753-16-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure-activity relationships of p-arylthio cinnamides as antagonists of LFA-1/ICAM-1)

RN 280753-11-9 CAPLUS
CN Benzaldehyde, 3-chloro-4-hydroxy-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 280753-16-4 CAPLUS
CN Benzaldehyde, 4-hydroxy-2,3-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:651421 CAPLUS
DOCUMENT NUMBER: 135:211431
TITLE: Transition metal complexes, olefin polymerization catalysts containing them, and their manufacture
INVENTOR(S): Kobayashi, Satoshi; Hino, Takahiro
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001240611	A2	20010904	JP 2000-390704	20001222

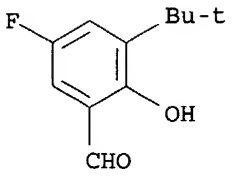
PRIORITY APPLN. INFO.: JP 1999-366990 A 19991224
OTHER SOURCE(S): MARPAT 135:211431
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The catalysts contain transition metal complexes I [R1-4, R6, R7 = H, halo, (un)substituted C1-20-hydrocarbon group, alkoxy, sulfonamide, imino, nitro, phosphino, thiophosphate group, etc.; R5 = H, C1-20-hydrocarbon group; X = halo, C1-20-hydrocarbon group, alkylthio, acyloxy, sulfonamide group, etc.; L = neutral ligand; M = IV-X group transition metal; p = 1-6; q ≥ 1; r, s = ≥0 (corresponding to valence of M)]. Thus, optically active Schiff base amino alc. II was reacted with TiCl4 in the presence of Et3N to give Ti complex III, which was mixed with methylaluminoxane to show catalyst activity 8.0 + 104 g/mol-Ti-h in ethylene polymerization

IT **357611-21-3P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(Schiff-base amino alc. transition metal complexes for olefin polymerization catalysts)

RN 357611-21-3 CAPLUS
CN Benzaldehyde, 3-(1,1-dimethylethyl)-5-fluoro-2-hydroxy- (9CI) (CA INDEX NAME)

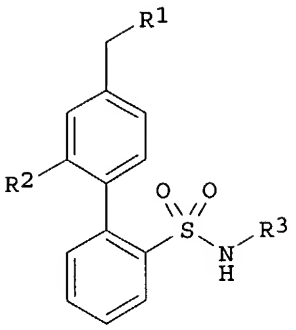


L22 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:453059 CAPLUS
DOCUMENT NUMBER: 135:46172
TITLE: Preparation of N-isoxazolyl biphenylsulfonamides and related compounds as dual angiotensin II and endothelin receptor antagonists.
INVENTOR(S): Murugesan, Natesan; Tellew, John E.; Macor, John E.; Gu, Zhengxiang
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: PCT Int. Appl., 287 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044239	A2	20010621	WO 2000-US33730	20001213
WO 2001044239	A3	20011101		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1237888	A2	20020911	EP 2000-984282	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520785	T2	20030708	JP 2001-544729	20001213

PRIORITY APPLN. INFO.:
US 1999-464037 A 19991215
US 2000-481197 A 20000111
US 2000-513779 A 20000225
US 2000-604322 A 20000626
US 2000-643640 A 20000822
WO 2000-US33730 W 20001213

OTHER SOURCE(S): MARPAT 135:46172
GI



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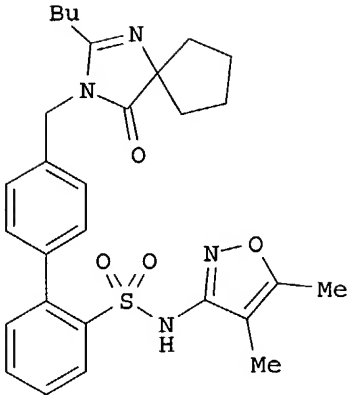


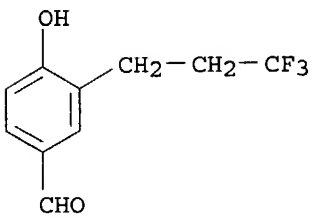
II

AB Title compds. (I; R1 = specified oxoimidazolyl, pyridoimidazolyl, pyridylamino, triazolyl, quinolinyloxy, etc.; R2 = H, halo, CHO, (halo)alkyl, cycloalkylalkyl, alkenyl, alkynyl, alkoxyalkyl, alkoxy, cyano, OH, NO2, etc.; R3 = heteroaryl; with provisos) were prepared as dual angiotensin II and endothelin receptor antagonists for treatment of hypertension and other diseases (no data). Thus, 4-BrC6H4CH2OH was coupled with [2-[[(4,5-dimethyl-3-isoxazolyl)[(2-methoxyethoxy)methyl]amino]sulfonyl]phenyl]boronic acid to give N-(4,5-dimethyl-3-isoxazolyl)-4'-(hydroxymethyl)-N-[(2-methoxyethoxy)methyl][1,1'-biphenyl]-2-sulfonamide (66%). This was brominated to give the 4'-bromomethyl derivative (90%), reacted with 2-butyl-1,3-diazaspiro[4.4]non-1-en-4-one hydrochloride, and deprotected (49% for two steps) to give II.

IT **254745-93-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-isoxazolyl biphenylsulfonamides and related compds. as dual angiotensin II and endothelin receptor antagonists)

RN 254745-93-2 CAPLUS

CN Benzaldehyde, 4-hydroxy-3-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:112487 CAPLUS

DOCUMENT NUMBER: 134:326325

TITLE: High Enantioselectivities in an (E)-Alkene Epoxidation by Catalytically Active Chromium Salen Complexes. Insight into the Catalytic Cycle

AUTHOR(S): Daly, Adrian M.; Renehan, Marie F.; Gilheany, Declan G.

CORPORATE SOURCE: Chemistry Department and Conway Institute of Biomolecular and Biomedical Sciences, University College Dublin, Belfield Dublin, Ire.

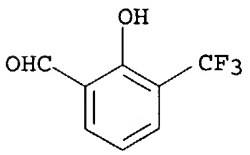
SOURCE: Organic Letters (2001), 3(5), 663-666

CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:326325

AB The epoxidn. of (E)-β-methylstyrene mediated by an oxochromium salen complex yields the epoxide in 92% ee in stoichiometric mode, the highest ee yet reported for a metal-mediated epoxidn. of an (E)-alkene. The effect of added donor ligands, previously substantial, has reached a ceiling with this complex. In catalytic mode a slightly reduced ee and higher yield is obtained, indicating both the presence of a second oxidation cycle and that the major oxidant reacts with its reduced form.

IT **336628-67-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective epoxidn. of β-methylstyrene by a chromium salen complex)

RN 336628-67-2 CAPLUS
CN Benzaldehyde, 2-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:725609 CAPLUS
DOCUMENT NUMBER: 133:296281
TITLE: Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Thomas W.; Winn, Martin; Xin, Zhili; Wang, Sheldon; Boyd, Steven A.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.; Jae, Hwan-soo; Lynch, John K.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 476 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

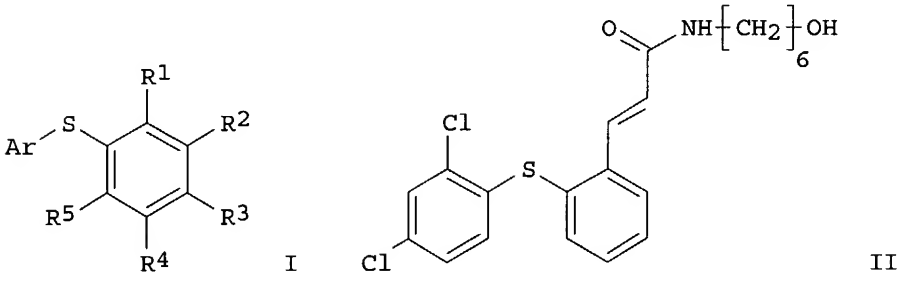
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059880	A1	20001012	WO 2000-US8895	20000403

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1165505		A1	20020102	EP 2000-921654		20000403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO						
BR 2000009426		A	20020409	BR 2000-9426		20000403
EE 200100513		A	20021216	EE 2001-513		20000403
JP 2004513063		T2	20040430	JP 2000-609392		20000403
NO 2001004767		A	20011130	NO 2001-4767		20011001
BG 106029		A	20020531	BG 2001-106029		20011018
HR 2001000776		A1	20021231	HR 2001-776		20011023
ZA 2001008944		A	20030702	ZA 2001-8944		20011030
PRIORITY APPLN. INFO.:				US 1999-286645	A	19990402
				US 1999-474517	A	19991229
				US 2000-541795	A	20000331
				WO 2000-US8895	W	20000403

OTHER SOURCE(S): MARPAT 133:296281

GI

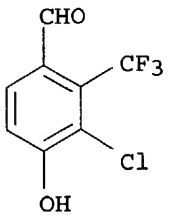


AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases. Examples include syntheses for 443 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp.

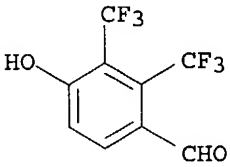
IT **280753-11-9P**, 3-Chloro-4-hydroxy-2-(trifluoromethyl)benzaldehyde
280753-16-4P, 4-Hydroxy-2,3-bis(trifluoromethyl)benzaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280753-11-9 CAPLUS

CN Benzaldehyde, 3-chloro-4-hydroxy-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 280753-16-4 CAPLUS
CN Benzaldehyde, 4-hydroxy-2,3-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:457022 CAPLUS
DOCUMENT NUMBER: 133:89514
TITLE: Cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Tom; Winn, Martin; Xin, Zhili; Boyd, Steven A.; Jae, Hwan-Soo; Lynch, John K.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 400 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039081	A2	20000706	WO 1999-US31162	19991229
WO 2000039081	A3	20010525		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6110922	A	20000829	US 1998-222491	19981229
CA 2356320	AA	20000706	CA 1999-2356320	19991229
EP 1140814	A2	20011010	EP 1999-966709	19991229
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533434	T2	20021008	JP 2000-590994	19991229

EE 200100355	A	20021015	EE 2001-355		19991229
NZ 512687	A	20031219	NZ 1999-512687		19991229
AU 771126	B2	20040311	AU 2000-22203		19991229
NO 2001003241	A	20010828	NO 2001-3241		20010628
HR 2001000512	A1	20020831	HR 2001-512		20010710
BG 105732	A	20020228	BG 2001-105732		20010725
PRIORITY APPLN. INFO.:			US 1998-222491	A	19981229
			WO 1999-US31162	W	19991229

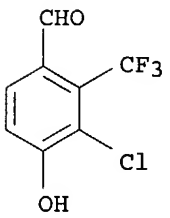
OTHER SOURCE(S): MARPAT 133:89514

AB The present invention relates to novel cinnamide compds. that are useful for treating inflammatory and immune diseases, to pharmaceutical compns. containing these compds., and to methods of inhibiting inflammation or suppressing immune response in a mammal. Among the approx. 400 trans-arylthiocinnamamide title compds., prepared by standard methods, were 6-benzodioxanyl 2-trifluoromethyl-4-[(E)-2-[3-(R)-(ethoxycarbonyl)piperidinocarbonyl]ethenyl]phenyl sulfide (I), 2-ethoxyphenyl 2-trifluoromethyl-4-[(E)-2-[2-carboxy-4-(methoxycarbonyl)-1-piperazinylcarbonyl]ethenyl]phenyl sulfide (II) and 2-isopropylphenyl 2-nitro-4-[(E)-2-[3-(2-oxo-1-pyrrolidinyl)-1-propylaminocarbonyl]ethenyl]phenyl sulfide (III). The abilities of the title compds. to antagonize the interaction between ICAM-1 and LFA-1 were quantified using both biochem. and cell-based adhesion assays. E.g., compds. I-III exhibited 98% inhibition @ 4μM.

IT **280753-11-9P**, 3-Chloro-4-hydroxy-2-trifluoromethylbenzaldehyde
280753-16-4P, 4-Hydroxy-2,3-bis(trifluoromethyl)benzaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(hetaryl)(arylthio)cinnamamides with antiinflammatory, immune suppressant and cell adhesion inhibiting activity)

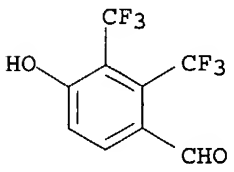
RN 280753-11-9 CAPLUS

CN Benzaldehyde, 3-chloro-4-hydroxy-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 280753-16-4 CAPLUS

CN Benzaldehyde, 4-hydroxy-2,3-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:34745 CAPLUS

DOCUMENT NUMBER: 132:93309

TITLE: Preparation of N-isoxazolyl biphenylsulfonamides and related compounds as dual angiotensin II and endothelin receptor antagonists.

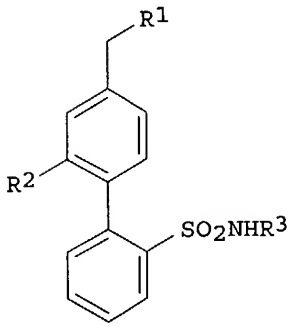
10/718,758

INVENTOR(S): Murugesan, Natesan; Tellew, John E.; Macor, John E.; Gu, Zhengxiang
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: PCT Int. Appl., 283 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000001389	A1	20000113	WO 1999-US15063	19990701
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2336714	AA	20000113	CA 1999-2336714	19990701
AU 9950888	A1	20000124	AU 1999-50888	19990701
AU 767456	B2	20031113		
EP 1094816	A1	20010502	EP 1999-935406	19990701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9911621	A	20011016	BR 1999-11621	19990701
TR 200100149	T2	20011022	TR 2001-200100149	19990701
EE 200100006	A	20020617	EE 2001-6	19990701
JP 2002519380	T2	20020702	JP 2000-557835	19990701
NZ 508118	A	20030725	NZ 1999-508118	19990701
ZA 2000006772	A	20020220	ZA 2000-6772	20001120
LT 4854	B	20011126	LT 2000-123	20001222
NO 2001000062	A	20010305	NO 2001-62	20010105
BG 105205	A	20010928	BG 2001-105205	20010131
LV 12639	B	20010920	LV 2001-17	20010205

PRIORITY APPLN. INFO.: US 1998-91847P P 19980706
WO 1999-US15063 W 19990701

OTHER SOURCE(S): MARPAT 132:93309
GI



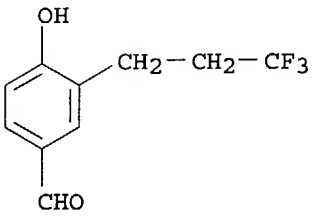
I

AB Title compds. (I; R1 = specified oxoimidazolyl, pyridoimidazolyl, pyridylamino, triazolyl, quinolinyloxy, etc.; R2 = H, halo, CHO, alkyl, haloalkyl, cycloalkylalkyl, alkenyl, alkynyl, alkoxyalkyl, alkoxy, cyano,

OH, NO2, etc.; R3 = heteroaryl; with provisos), were prepared as dual angiotensin II and endothelin receptor antagonists (no data). Thus, 4-BrC6H4CH2OH was coupled with [2-[[(4,5-dimethyl-3-isoxazolyl)[(2-methoxyethoxy)methyl]amino]sulfonyl]phenyl]boronic acid to give N-(4,5-dimethyl-3-isoxazolyl)-4'-(hydroxymethyl)-N-[(2-methoxyethoxy)methyl][1,1'-biphenyl]-2-sulfonamide. This was brominated to give 4'-bromomethyl-N-(4,5-dimethyl-3-isoxazolyl)-N-[(2-methoxyethoxy)methyl][1,1'-biphenyl]-2-sulfonamide, which reacted with 2-butyl-1,3-diazaspiro[4.4]non-1-en-4-one hydrochloride followed by deprotection to give 4'-[(2-butyl-4-oxo-1,3-diazaspiro[4.4]non-1-en-3-yl)methyl]-N-(4,5-dimethyl-3-isoxazolyl)[1,1'-biphenyl]-2-sulfonamide.

IT **254745-93-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-isoxazolyl biphenylsulfonamides and related compds. as dual angiotensin II and endothelin receptor antagonists)

RN 254745-93-2 CAPLUS
CN Benzaldehyde, 4-hydroxy-3-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



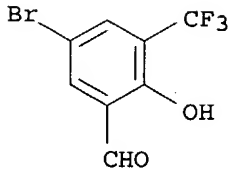
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:727406 CAPLUS
DOCUMENT NUMBER: 132:3235
TITLE: An improved method for the synthesis of 3-fluorosalicylic acid with application to the synthesis of 3-(trifluoromethyl)salicylic acid
AUTHOR(S): Micklatcher, Mark L.; Cushman, Mark
CORPORATE SOURCE: Dep. Medicinal Chem. Molecular Pharmacology, School Pharmacy Pharmacal Sciences, Purdue Univ., West Lafayette, IN, 47907, USA
SOURCE: Synthesis (1999), (11), 1878-1880
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:3235

AB An improved method for the synthesis of 3-fluorosalicylic acid is described. A positional protective group strategy allows formylation selectively at the ortho position of 4-bromo-2-fluorophenol. Oxidation of the resulting salicylaldehyde to the salicylic acid, followed by debromination, affords 3-fluorosalicylic acid. The method has also been applied to the synthesis of 3-(trifluoromethyl)salicylic acid.

IT **251300-30-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluoro- and (fluoromethyl)salicylate)

RN 251300-30-8 CAPLUS
CN Benzaldehyde, 5-bromo-2-hydroxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

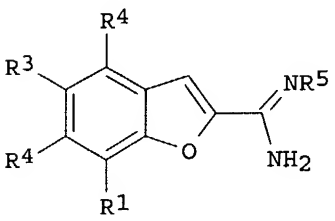


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:603140 CAPLUS
DOCUMENT NUMBER: 131:214186
TITLE: Preparation of benzofurancarboxamidines as central nervous system agents.
INVENTOR(S): Bos, Michael; Stadler, Heinz; Wichmann, Jurgen
PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5955495	A	19990921	US 1997-837140	19970414

PRIORITY APPLN. INFO.: US 1997-837140 19970414
OTHER SOURCE(S): MARPAT 131:214186
GI

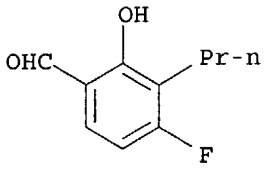


I

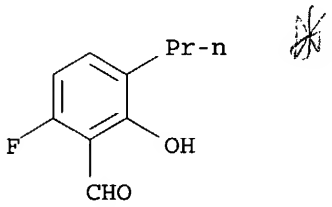
AB Title compds. (I; R1-R4 = H, halo, alkyl, alkoxy, aryl, benzyloxy, alkoxyalkyl, alkylsulfanyl, alkylsulphanylalkyl; R1R2 = OCH2CH2; R5 = H, OH) were prepared for treatment of migraine, schizophrenia, anxiety states, sleep disorders, anorexia, Alzheimer's disease, addictions, and disorders which result from damage to the head/brain or to the spinal column. Thus, 5,6-difluorobenzofuran-2-carboxamide (preparation given) was stirred 64 h with triethyloxonium tetrafluoroborate in CH2Cl2 to give a residue which was refluxed with NH4Cl in EtOH to give 40% 5,6-difluorobenzofuran-2-carboxamidine. The latter stimulated penile erection in rats with ID50 = 6.0 mg/kg orally.

IT **199287-71-3P 199287-80-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzofurancarboxamidines as central nervous system agents)

RN 199287-71-3 CAPLUS
CN Benzaldehyde, 4-fluoro-2-hydroxy-3-propyl- (9CI) (CA INDEX NAME)



RN 199287-80-4 CAPLUS
CN Benzaldehyde, 6-fluoro-2-hydroxy-3-propyl- (9CI) (CA INDEX NAME)



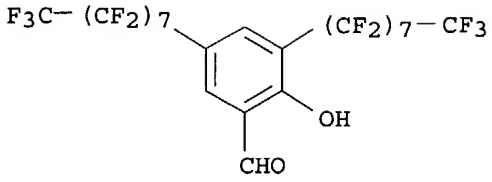
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:497083 CAPLUS
DOCUMENT NUMBER: 131:237131
TITLE: Enantioselective catalysis in fluorinated media. Synthesis and properties of chiral perfluoroalkylated (salen)manganese complexes
AUTHOR(S): Pozzi, Gianluca; Cavazzini, Marco; Cinato, Flavio; Montanari, Fernando; Quici, Silvio
CORPORATE SOURCE: Dipartimento Chimica Organica Industriale, Univ. Milano, Milan, I-20133, Italy
SOURCE: European Journal of Organic Chemistry (1999), (8), 1947-1955
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

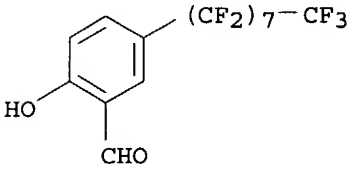
AB Chiral (salen)Mn complexes, which are selectively soluble in perfluorocarbons, were synthesized and tested as epoxidn. catalysts in fluorous-organic 2-phase systems. The immiscibility of the perfluorocarbons with regular organic solvents allowed a quick and effective separation of the catalyst from the products. These unprecedented perfluoroalkylated salen complexes were found to be efficient and chemoselective catalysts in the presence of several O donors, but enantioselectivities were generally poor. An interesting exception to this behavior was observed in the asym. epoxidn. of indene that provides indene oxide with 70-92% enantiomeric excess.

IT **207555-44-0P 244049-59-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of salen derivs. and its Mn complexes acting as epoxidn. catalysts)

RN 207555-44-0 CAPLUS
CN Benzaldehyde, 3,5-bis(heptadecafluorooctyl)-2-hydroxy- (9CI) (CA INDEX NAME)

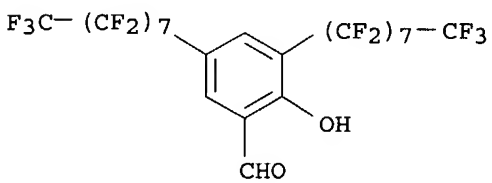


RN 244049-59-0 CAPLUS
CN Benzaldehyde, 5-(heptadecafluorooctyl)-2-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:259699 CAPLUS
DOCUMENT NUMBER: 129:4531
TITLE: Efficient aerobic epoxidation of alkenes in perfluorinated solvents catalyzed by chiral (salen) Mn complexes
AUTHOR(S): Pozzi, Gianluca; Cinato, Flavio
CORPORATE SOURCE: Centro CNR and Dipartimento di Chimica Organica e Industriale dell'Universita, Milan, I-20133, Italy
SOURCE: Chemical Communications (Cambridge) (1998), (8), 877-878
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:4531
AB Chiral complexes selectively soluble in perfluorocarbons have been synthesized for the first time and tested as catalysts for the epoxidn. of alkenes under fluorous biphasic conditions.
IT **207555-44-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(efficient aerobic epoxidn. of alkenes in perfluorinated solvents catalyzed by chiral (salen) Mn complexes)
RN 207555-44-0 CAPLUS
CN Benzaldehyde, 3,5-bis(heptadecafluorooctyl)-2-hydroxy- (9CI) (CA INDEX NAME)



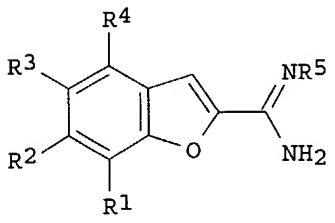
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:746041 CAPLUS
DOCUMENT NUMBER: 128:22807
TITLE: Benzofuryl derivatives and their use
INVENTOR(S): Bos, Michael; Stadler, Heinz; Wichmann, Jurgen
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9742183	A1	19971113	WO 1997-EP2092	19970424
W: AU, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, NZ, PL, RU, SG, TR, YU				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9727696	A1	19971126	AU 1997-27696	19970424
AU 712056	B2	19991028		
EP 906301	A1	19990407	EP 1997-921737	19970424
EP 906301	B1	20021002		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1217720	A	19990526	CN 1997-194357	19970424
JP 11508283	T2	19990721	JP 1997-539479	19970424
JP 3148253	B2	20010319		
BR 9708902	A	19990803	BR 1997-8902	19970424
TR 9802206	T2	20011221	TR 1998-9802206	19970424
AT 225342	E	20021015	AT 1997-921737	19970424
PT 906301	T	20030228	PT 1997-921737	19970424
ES 2182070	T3	20030301	ES 1997-921737	19970424
ZA 9703708	A	19971103	ZA 1997-3708	19970429
KR 2000010708	A	20000225	KR 1998-708809	19981102

PRIORITY APPLN. INFO.: EP 1996-106990 A 19960503
WO 1997-EP2092 W 19970424

OTHER SOURCE(S): MARPAT 128:22807
GI

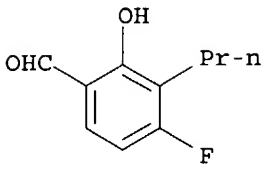


I

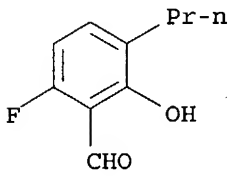
AB Title compds. I (R1-R4 = H, halo, alkyl, alkoxy, aryl, benzyloxy, alkylthio, etc.; R5 = H, OH) were prepared from benzo[b]furan-2-carboxamides or -2-carbonitriles. Affinities to the 5-HT2C and 5-HT2A receptors were determined and the results expressed as pKi values, e.g., I (R1 = R2 = R4 = R5 = H, R3 = F) had pKi values of 6.8 and 5.7 for the above receptors, resp.

IT **199287-71-3P 199287-80-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzofuryl derivs. and their affinity to 5-HT2C and 5-HT2A receptors)

RN 199287-71-3 CAPLUS
CN Benzaldehyde, 4-fluoro-2-hydroxy-3-propyl- (9CI) (CA INDEX NAME)



RN 199287-80-4 CAPLUS
CN Benzaldehyde, 6-fluoro-2-hydroxy-3-propyl- (9CI) (CA INDEX NAME)



L22 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:204149 CAPLUS
DOCUMENT NUMBER: 126:199573
TITLE: Heterocyclylcarboxamide derivatives for use as neurotransmitter agonists
INVENTOR(S): Birch, Alan Martin; Heal, David John; Kerrigan, Frank; Martin, Keith Frank; Needham, Patricia Lesley; Sargent, Bruce Jeremy
PATENT ASSIGNEE(S): Knoll Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

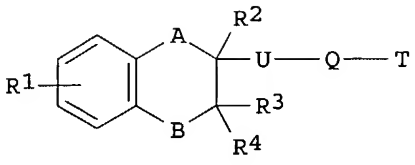
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9703071	A1	19970130	WO 1996-EP2890	19960702
W: AU, BG, BR, CA, CN, CZ, GE, HU, IL, JP, KR, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2223472	AA	19970130	CA 1996-2223472	19960702
AU 9665172	A1	19970210	AU 1996-65172	19960702
AU 708890	B2	19990812		
EP 839145	A1	19980506	EP 1996-924847	19960702
EP 839145	B1	20031105		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LV, FI				
CN 1190967	A	19980819	CN 1996-195477	19960702
CN 1071755	B	20010926		
BR 9609506	A	19990601	BR 1996-9506	19960702
JP 11508599	T2	19990727	JP 1996-505471	19960702
RU 2169147	C2	20010620	RU 1998-102441	19960702
IL 122540	A1	20011031	IL 1996-122540	19960702
AT 253573	E	20031115	AT 1996-924847	19960702
ZA 9605921	A	19980112	ZA 1996-5921	19960712
TW 454006	B	20010911	TW 1996-85115692	19961219
US 5935973	A	19990810	US 1998-981671	19980105
NO 9800129	A	19980112	NO 1998-129	19980112

PRIORITY APPLN. INFO.: GB 1995-14380 A 19950713

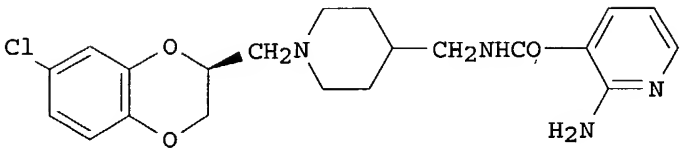
WO 1996-EP2890 W 19960702

OTHER SOURCE(S): MARPAT 126:199573

GI



I



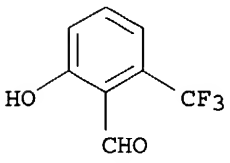
II

AB Title compds. I [A, B = CH2, O; R1 = optional substituent(s); R2-R4 = H, (un)substituted alkyl; U = (un)branched alkylene; Q = N-containing divalent group; T = heterocyclylcarbonyl attached to N in Q] were prepared for use in treating central nervous system disorders. Thus, the benzodioxane II was prepared from 5-chloro-2-hydroxybenzaldehyde, (R)-glycidyl tosylate, and 4-aminomethylpiperidine in 8 steps. II had a Ki for 5 HT1α receptor binding of 41.5 nM and also bound to the α2D, D2, and α1 receptors.

IT **58914-35-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzodioxanylmethylpiperidinylmethylcarbamoylpyridines as neurotransmitter agonists)

RN 58914-35-5 CAPLUS

CN Benzaldehyde, 2-hydroxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:314282 CAPLUS

DOCUMENT NUMBER: 120:314282

TITLE: Complexes with macrocyclic ligands. I. Dinuclear copper(II) complexes with a totally π-conjugated macrocycle of Schiff base type: syntheses, structures, electro-, and magnetochemical properties

AUTHOR(S): Brychcy, Klaus; Drager, Klaus; Jens, Klaus J.; Tilset, Mats; Behrens, Ulrich

CORPORATE SOURCE: Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, 20146, Germany

SOURCE: Chemische Berichte (1994), 127(3), 465-76
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

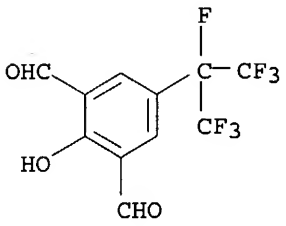
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB [Cu2L](ClO4)2 (H2L = I (R = CMe3, X = H, F; R = (CF3)2CF, X = F)) (II, III and IV, resp,) were synthesized by the Schiff base condensation of 2 equiv of 1,2-phenylenediamines and 2,6-diformylphenols in the presence of 2 equiv of Cu(ClO4)2 and were characterized by x-ray structure analyses, electrochem. studies (DCV), and variable-temperature magnetic susceptibility measurements. II exists in 2 different solvated crystalline forms. The Cu(II) ions in all 3 complexes are octahedrally coordinated with long axial distances to solvent mols. or perchlorate ions. The Cu ions in II (in solvate a) are only five-coordinate and square-pyramidal. The CuIICuII complexes were reduced in successive, quasi-reversible, 1-electron steps. The antiferromagnetic exchange interactions were determined Upon dissoln. in MeCN IV decomposed to form [Cu(MeCN)4]ClO4 and V (x-ray structure determination).

IT **154853-68-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenylenediamines in presence of copper perchlorate)

RN 154853-68-6 CAPLUS

CN 1,3-Benzenedicarboxaldehyde, 2-hydroxy-5-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

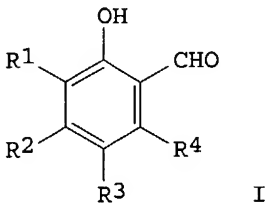


L22 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:574212 CAPLUS
DOCUMENT NUMBER: 119:174212
TITLE: Substituted salicylaldehydes as glucose-6-phosphatase-inhibiting drugs.
INVENTOR(S): Below, Peter; Herling, Andreas; Rippel, Robert; Schindler, Peter
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4202184	A1	19930729	DE 1992-4202184	19920128

PRIORITY APPLN. INFO.: DE 1992-4202184 19920128

OTHER SOURCE(S): MARPAT 119:174212
GI



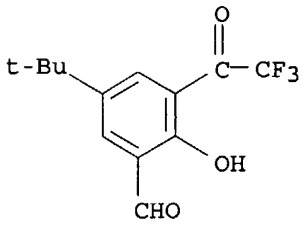
I

AB The salicylaldehydes I (R1, R2 = NO2, CN, CHO, CO2H, alkoxycarbonyl, CONH2, etc.; R3, R4 = H, F, Cl, Br, alkyl, alkoxy; R2R4 = alkylene) are inhibitors of glucose 6-phosphatase (II) and gluconeogenesis, useful i.a. for treatment of type II diabetes. I (R1 = NO2, R3 = tert-Bu, R2 = R4 = H) (91 μM) inhibited II by 50%, in vitro. Formulation examples are given.

IT **150023-28-2**
RL: BIOL (Biological study)
(glucose phosphatase inhibition by, as antidiabetic drug)

RN 150023-28-2 CAPLUS

CN Benzaldehyde, 5-(1,1-dimethylethyl)-2-hydroxy-3-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

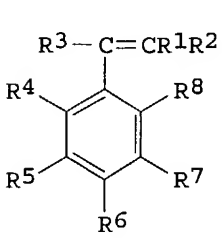


L22 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:516977 CAPLUS
DOCUMENT NUMBER: 119:116977
TITLE: Preparation and use of styrene derivatives as neoplasm inhibitors
INVENTOR(S): Kitano, Yasunori; Takayanagi, Hisao; Sugawara, Koichi; Hara, Hiroto; Nakamura, Hideo; Oshino, Toshiko
PATENT ASSIGNEE(S): Mitsubishi Kasei Corp., Japan
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

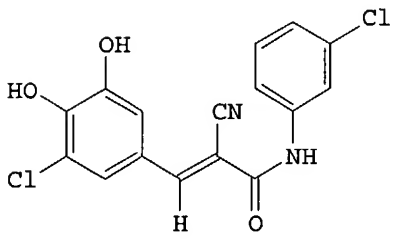
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 537742	A2	19930421	EP 1992-117632	19921015
EP 537742	A3	19930512		
EP 537742	B1	19960821		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 05301838	A2	19931116	JP 1992-266027	19921005
CA 2080554	AA	19930416	CA 1992-2080554	19921014
ES 2093753	T3	19970101	ES 1992-117632	19921015

US 5514711	A	19960507	US 1995-369263	19950105
PRIORITY APPLN. INFO.:			JP 1991-266461	19911015
			JP 1992-266027	19921005
			US 1992-961315	19921015

OTHER SOURCE(S): MARPAT 119:116977
GI



I



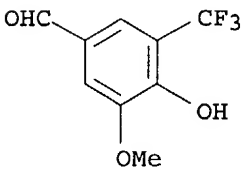
II

AB Styrene derivs. I (R1, R2 = cyano, amido, etc., R3 = alkyl, hydroxy; R4-8 = H, hydroxy, halo, etc.) and pharmaceuticals containing them are claimed. I are tyrosine kinase inhibitors and anticancer agents. For example, N-(3-chlorophenyl)-2-cyano-3-(3-chloro-4,5-dihydroxyphenyl)propenamide (II) was prepared from 5-chlorovanillin and N-(3-chlorophenyl)cyanoacetamide. For II the tyrosine kinase inhibitory IC50 was 0.68 μM and II at 1000 mg/kg was not toxic in mice.

IT **116314-60-4**, 3-Methoxy-4-hydroxy-5-(trifluoromethyl)benzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for styrene derivative (neoplasm inhibitor, tyrosine kinase inhibitor))

RN 116314-60-4 CAPLUS

CN Benzaldehyde, 4-hydroxy-3-methoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

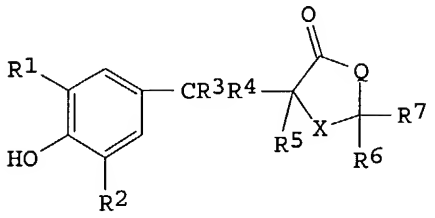
ACCESSION NUMBER:	1993:6969 CAPLUS
DOCUMENT NUMBER:	118:6969
TITLE:	Preparation of aryl-substituted rhodanine derivatives for the treatment of type I diabetes
INVENTOR(S):	Lafferty, Kevin John; Panetta, Jill Ann
PATENT ASSIGNEE(S):	University of Colorado Foundation, Inc., USA
SOURCE:	Eur. Pat. Appl., 45 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 500337	A1	19920826	EP 1992-301351	19920219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE				
US 5158966	A	19921027	US 1991-660328	19910222

ZA 9201108	A	19930814	ZA 1992-1108	19920214
CA 2061363	AA	19920823	CA 1992-2061363	19920217
AU 9211114	A1	19920827	AU 1992-11114	19920220
AU 651865	B2	19940804		
HU 66536	A2	19941228	HU 1992-549	19920220
JP 06048943	A2	19940222	JP 1992-34838	19920221

PRIORITY APPLN. INFO.: US 1991-660328 19910222
OTHER SOURCE(S): MARPAT 118:6969
GI

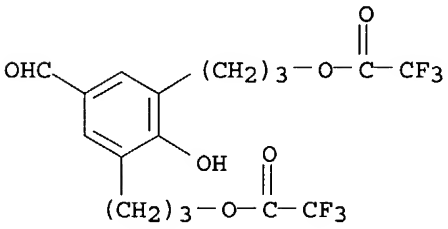


I

AB Title compds. I (R1, R2 = H, C1-6 alkyl, C1-6 alkoxy, C2-6 alkenyl, C2-6 alkynyl, C1-4-alkyl-O2C-C14-alkyl, PhS(CH2)n; n = 0-3; R3 = H, C1-6 alkyl; R4, R5 = H, R4R5 = bond; R6, R7 = H, or when one of R6, R7 = H the other is HO, MeS; R6R7 = S, O; X = S(O)m wherein m = 0-2; Q = CH2, O, R8N wherein R8 = H, C1-6 alkyl, C2-6 alkenyl, etc.) are prepared 3,5,4-(Me3C)2(HO)C6H2CHO, rhodamine, and fused NaOAc were refluxed to give I (R1 = R2 = Me3C, R3 = R4 = R5 = H, R6R7 = X = S) (II). II in EtOH was hydrogenated in presence of Pd/C to give I (R1 = R2 = Me3C, R3-R7 = H, Q = HN, X = S) (III). Mice given 250 mg/kg cyclophosphamide (IV) and fed a diet containing 0.1 weight% III one day prior to IV and continued for 21 days, resulted in 5/17 animals developing diabetes. Pharmaceutical formulations comprising I are given.

IT **132392-93-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antidiabetic)

RN 132392-93-9 CAPLUS
CN Acetic acid, trifluoro-, (5-formyl-2-hydroxy-1,3-phenylene)di-3,1-propanediyl ester (9CI) (CA INDEX NAME)

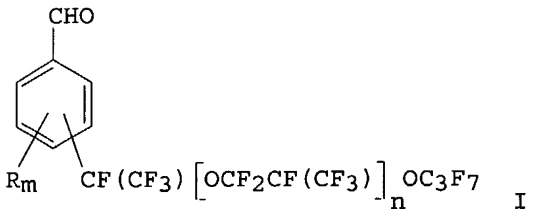


L22 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:489941 CAPLUS
DOCUMENT NUMBER: 117:89941
TITLE: Preparation of polyfluoroalkyl group containing aromatic aldehyde derivatives
INVENTOR(S): Mitani, Motohiro; Sawada, Hideo; Nakayama, Masaharu
PATENT ASSIGNEE(S): Nippon Yushi K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04082855	A2	19920316	JP 1990-194783	19900725

PRIORITY APPLN. INFO.: JP 1990-194783 19900725
OTHER SOURCE(S): CASREACT 117:89941; MARPAT 117:89941
GI

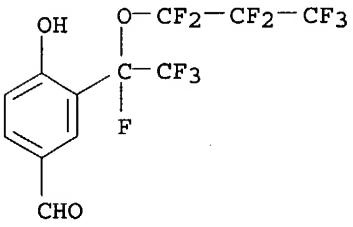


I

AB The title derivs. I (R = CO2H, OH, halo, C1-4 alkyl, C1-4 alkoxy, C1-4 alkoxycarbonyl, C1-4 alkanesulfonyl; m = 0-4; n = 0-8) are prepared by treating C3F7O[CF(CF3)CF2O]nCF(CF3)CO2OCOCF(CF3)[OCF2CF(CF3)]nOC3F7 (II) with RmC6H5-mCHO. A solution of II (n = 0) in 1,1,2-trichlorotrifluoroethane was treated with PhCHO at 40° for 5 h to give 90% I (m = 0).

IT **142808-05-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by perfluoroalkylation of benzaldehydes)

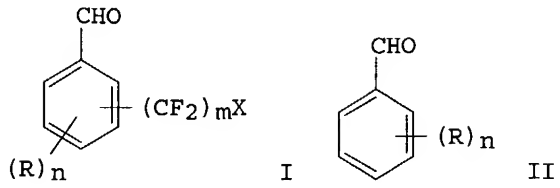
RN 142808-05-7 CAPLUS
CN Benzaldehyde, 4-hydroxy-3-[1,2,2,2-tetrafluoro-1-(heptafluoropropoxy)ethyl]- (9CI) (CA INDEX NAME)



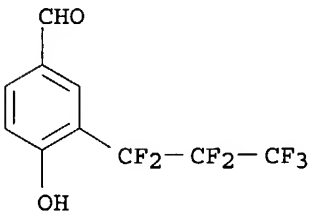
L22 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:607657 CAPLUS
DOCUMENT NUMBER: 115:207657
TITLE: Manufacture of fluorine-containing benzaldehyde derivatives
INVENTOR(S): Mitani, Motohiro; Sawada, Hideo; Nakayama, Masaharu
PATENT ASSIGNEE(S): Nippon Oil and Fats Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 03123751 A2 19910527 JP 1989-260200 19891006
PRIORITY APPLN. INFO.: JP 1989-260200 19891006
OTHER SOURCE(S): CASREACT 115:207657; MARPAT 115:207657
GI



AB Title derivs. I (R = halo, C1-4 alkyl, C1-4 alkoxy, C1-4 alkoxycarbonyl, CO2H, OH, C1-4 alkanesulfonyl; X = F, Cl, H; m = 1-10; n = 0-4; m = 10 when n = 0 or 1 and R = halo) are manufactured by the reaction of benzaldehydes II with X(F2C)mCOO2CO(CF2)mX. Thus, treating benzaldehyde with bis(heptafluorobutyryl) peroxide in 1,1,2-trichlorotrifluoroethane at 40° under N gave 90% 3-heptafluoropropylbenzaldehyde.
IT **136850-61-8P**, 3-Heptafluoropropyl-4-hydroxybenzaldehyde
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by perfluoroalkylation with bis(heptafluorobutyryl) peroxide)
RN 136850-61-8 CAPLUS
CN Benzaldehyde, 3-(heptafluoropropyl)-4-hydroxy- (9CI) (CA INDEX NAME)



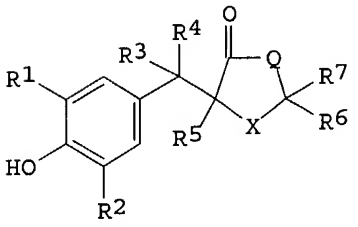
L22 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:122357 CAPLUS
DOCUMENT NUMBER: 114:122357
TITLE: Preparation of 5-(4-hydroxyphenyl)-2-thioxo-4-thiazolidinones and related compounds as antinflammatories
INVENTOR(S): Panetta, Jill Ann
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 69 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 391644	A2	19901010	EP 1990-303510	19900402
EP 391644	A3	19910424		
EP 391644	B1	19960619		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
CA 2013599	AA	19901007	CA 1990-2013599	19900402

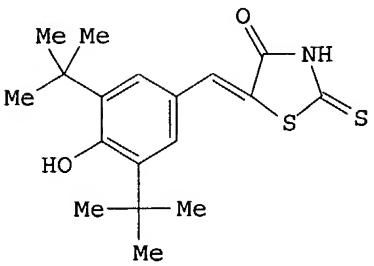
CA 2013599	C	19991116			
ZA 9002520	A	19911224	ZA 1990-2520		19900402
AT 139531	E	19960715	AT 1990-303510		19900402
ES 2088965	T3	19961001	ES 1990-303510		19900402
AU 9052934	A1	19901011	AU 1990-52934		19900405
AU 629322	B2	19921001			
JP 02290862	A2	19901130	JP 1990-92981		19900406
HU 56356	A2	19910828	HU 1990-2115		19900406
US 5356917	A	19941018	US 1993-111226		19930824
US 5691367	A	19971125	US 1996-733909		19961018
PRIORITY APPLN. INFO.:			US 1989-335063	A	19890407
			US 1985-764160	B2	19850809
			US 1986-869488	B1	19860602
			US 1987-114278	B1	19871027
			US 1989-304919	B2	19890201
			US 1990-504147	B1	19900403
			US 1992-839693	B1	19920220
			US 1993-111226	A3	19930824
			US 1994-290664	A1	19940815

OTHER SOURCE(S): MARPAT 114:122357

GI



I



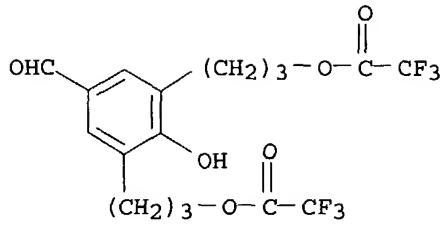
II

AB The title compds. (I; R1, R2 = H, alkyl, alkoxy, alkylcarbonyloxyalkyl; R3 = H, alkyl; R4, R5 = H; R4R5 = bond; R5, R6 = H, or one of R6,R7 = H, the other = OH, SMe; R5R6 = S, O; X = SOn; n = 0-2), were prepared Thus, a mixture of 3,5-di-tert-butyl-4-hydroxybenzaldehyde, rhodanine, and NaOAc was refluxed 23 h in HOAc to give title compound II. II at 50 mg/kg orally in rats gave 100% inhibition of collagen-induced arthritis. I also prevented ischemic-induced brain damage in rats and prolonged the lives of dystrophic mice. Pharmaceutical I formulations are given.

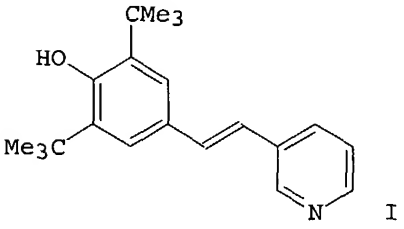
IT **132392-93-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (hydroxyphenylmethylene)thiazolidinone antiinflammatory)

RN 132392-93-9 CAPLUS

CN Acetic acid, trifluoro-, (5-formyl-2-hydroxy-1,3-phenylene)di-3,1-propanediyl ester (9CI) (CA INDEX NAME)



L22 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:423249 CAPLUS
DOCUMENT NUMBER: 113:23249
TITLE: Effect of structure on potency and selectivity in 2,6-disubstituted-4-(2-arylethenyl)phenol lipoxygenase inhibitors
AUTHOR(S): Lazer, Edward S.; Wong, Hin Chor; Wegner, Craig D.; Graham, Anne G.; Farina, Peter R.
CORPORATE SOURCE: Dep. Med. Chem., Boehringer Ingelheim Pharm., Inc., Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (1990), 33(7), 1892-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23249
GI

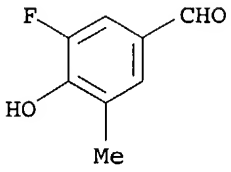


I

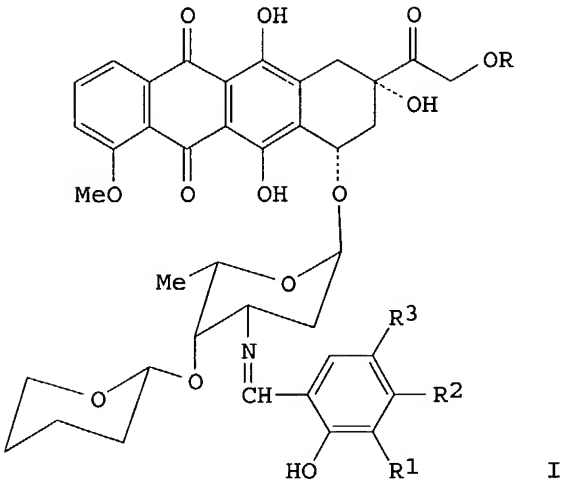
AB A series of 2,6-disubstituted 4-(2-arylethenyl)phenols with potent human PMN 5-lipoxygenase (5-LO) inhibiting activity (IC50s in the 10-7 M range) and weaker human platelet cyclooxygenase (CO) inhibiting activity (IC50s in the 10-6 M range) is described. This series evolved from the chemical modification of an antiinflammatory dual CO/5-LO inhibitor, 2,6-di-tert-butyl-4-[2-(3-pyridyl)ethenyl]phenol (I). The potency and selectivity for 5-LO inhibition is greatly influenced by the nature of the substituents in the 2- and 6-positions. Other structure-activity relationships that determine relative 5-LO and CO potency are discussed. In vivo activity against antigen-induced leukotriene-mediated bronchoconstriction and cell influx in guinea pigs is presented. Representatives of the series are active when administered at 30 mg/kg i.p.

IT **127036-07-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with arylacetic acid)

RN 127036-07-1 CAPLUS
CN Benzaldehyde, 3-fluoro-4-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



L22 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:179668 CAPLUS
DOCUMENT NUMBER: 112:179668
TITLE: N-Salicylidene derivatives of pirarubicin
AUTHOR(S): Ajito, Keiichi; Ikeda, Daishiro; Komuro, Keiko; Nosaka, Chisato; Wako, Nobuko; Kondo, Shinichi; Takeuchi, Tomio
CORPORATE SOURCE: Inst. Microbial Chem., Tokyo, 141, Japan
SOURCE: Journal of Antibiotics (1989), 42(7), 1133-44
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:179668
GI



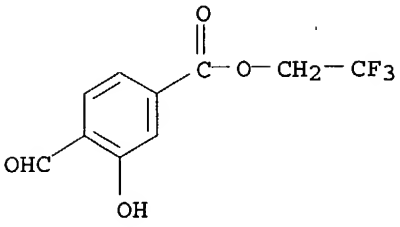
I

AB The preparation and biol. evaluation of N-salicylidene derivs. I (R = H, CO(CH2)4Me, CO(CH2)8Me; R1 = H, OH; R2 = H, OH, OMe, CO2Me, etc.; R3 = H, OH, OMe; 16 compds.] of pirarubicin are described. Pirarubicin was treated with various kinds of aryl aldehydes. Most of compds. synthesized here were more active than pirarubicin in vitro. Some of them showed significant prolongation of the survival period in exptl. mice by oral administration. Interestingly, a derivative containing forphenicine exhibited the broadest dose-response range by i.p. administration.

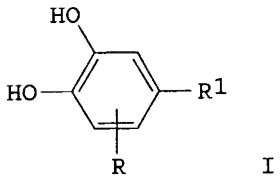
IT **126200-20-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with pirarubicin)

RN 126200-20-2 CAPLUS
CN Benzoic acid, 4-formyl-3-hydroxy-, 2,2,2-trifluoroethyl ester (9CI) (CA

INDEX NAME)



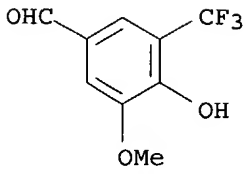
L22 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:172835 CAPLUS
DOCUMENT NUMBER: 110:172835
TITLE: Synthesis of some novel potent and selective catechol O-methyltransferase inhibitors
AUTHOR(S): Backstrom, Reijo; Honkanen, Erkki; Pippuri, Aino; Kairisalo, Pekka; Pystynen, Jarmo; Heinola, Kalevi; Nissinen, Erkki; Linden, Inge Britt; Mannisto, Pekka T.; et al.
CORPORATE SOURCE: Orion Pharm. Res. Lab., Orion Corp., Espoo, SF-02101, Finland
SOURCE: Journal of Medicinal Chemistry (1989), 32(4), 841-6
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:172835
GI



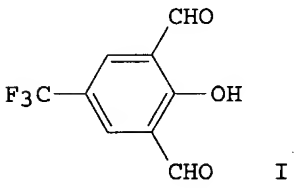
I

AB A series of disubstituted catechol derivs., e.g. I (R = NO2, CF3, CHO, Cl; R1 = Cl, NO2, cyano, CHO) was synthesized and tested as potential catechol O-methyltransferase (COMT) inhibitors. The most active compds. were more than 1000 times more potent (IC50 = 3-6 nM) in vitro than the known COMT inhibitor, 3',4'-dihydroxy-2-methylpropiophenone (U 0521, IC50 = 6000 nM). The new compds. were also highly selective COMT inhibitors with no activity against other essential enzymes involved in the synthesis and metabolism of catecholamines.

IT **116314-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)
RN 116314-60-4 CAPLUS
CN Benzaldehyde, 4-hydroxy-3-methoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



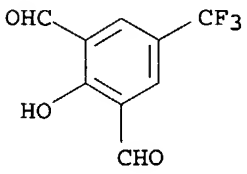
L22 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:74967 CAPLUS
DOCUMENT NUMBER: 110:74967
TITLE: Synthesis of 2,6-diformyl-4-trifluoromethylphenol
AUTHOR(S): Leroy, Jacques; Wakselman, Claude; Lacroix, Pascal; Kahn, Olivier
CORPORATE SOURCE: C.E.R.C.O.A, C.N.R.S., Thiais, F-94320, Fr.
SOURCE: Journal of Fluorine Chemistry (1988), 40(1), 23-32
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:74967
GI



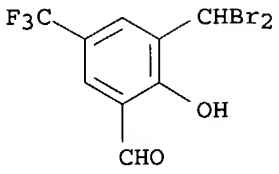
AB A convenient method for preparation of the previously unknown title compound (I)
by a seven-stage synthesis is reported. A Me ether is used to protect the phenol moiety and the key step involves a copper-mediated trifluoromethylation of a bromoanisole prepared from 4-BrC6H4OH.

IT **114315-20-7P**, 2,6-Diformyl-4-(trifluoromethyl)phenol
118745-73-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 114315-20-7 CAPLUS
CN 1,3-Benzenedicarboxaldehyde, 2-hydroxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 118745-73-6 CAPLUS
CN Benzaldehyde, 3-(dibromomethyl)-2-hydroxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:528570 CAPLUS
DOCUMENT NUMBER: 109:128570
TITLE: Preparation of pyrocatechol derivatives for treating Parkinson's disease
INVENTOR(S): Backstrom, Reijo Johannes; Heinola, Kalevi Evert; Honkanen, Erkki Juhani; Kaakkola, Seppo Kalevi; Kairisalo, Pekka Juhani; Linden, Inge Britt Yvonne; Mannistoe, Pekka Topias; Nissinen, Erkki Aarne Olavi; Pohto, Pentti; et al.
PATENT ASSIGNEE(S): Orion-Yhtyma Oy, Finland
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3740383	A1	19880601	DE 1987-3740383	19871127
DE 3740383	C2	19970925		
CN 87108011	A	19880608	CN 1987-108011	19871126
CN 1040062	B	19981007		
DK 8706230	A	19880529	DK 1987-6230	19871127
FI 8705229	A	19880529	FI 1987-5229	19871127
FI 93350	B	19941215		
FI 93350	C	19950327		
SE 8704751	A	19880529	SE 1987-4751	19871127
SE 503434	C2	19960617		
NO 8704966	A	19880530	NO 1987-4966	19871127
NO 171450	B	19921207		
NO 171450	C	19930317		
AU 8781879	A1	19880602	AU 1987-81879	19871127
AU 621036	B2	19920305		
FR 2607493	A1	19880603	FR 1987-16457	19871127
FR 2607493	B1	19940812		
NL 8702857	A	19880616	NL 1987-2857	19871127
NL 194821	B	20021202		
NL 194821	C	20030403		
JP 63150237	A2	19880622	JP 1987-301387	19871127
JP 2735834	B2	19980402		
JP 63170311	A2	19880714	JP 1987-301388	19871127
JP 08005781	B4	19960124		
GB 2200109	A1	19880727	GB 1987-27854	19871127
GB 2200109	B2	19910703		
ZA 8708953	A	19880727	ZA 1987-8953	19871127
HU 45473	A2	19880728	HU 1987-5352	19871127
HU 206073	B	19920828		
ES 2008359	A6	19890716	ES 1987-3401	19871127
US 4963590	A	19901016	US 1987-126911	19871127
PL 152642	B1	19910131	PL 1987-269091	19871127
PL 154006	B1	19910628	PL 1987-283185	19871127

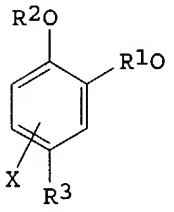
CA 1289078	A1	19910917	CA 1987-552986	19871127
BE 1003279	A5	19920218	BE 1987-1356	19871127
CS 276263	B6	19920513	CS 1988-8439	19871127
CS 277018	B6	19921118	CS 1988-8440	19871127
RU 2014319	C1	19940615	RU 1987-4203731	19871127
CA 1334967	A1	19950328	CA 1987-552987	19871127
CH 685436	A	19950714	CH 1987-4633	19871127
AT 8703129	A	19951015	AT 1987-3129	19871127
AT 401053	B	19960625		
DD 281375	A5	19900808	DD 1987-309670	19871130
SU 1729291	A3	19920423	SU 1989-4613317	19890123
US 5112861	A	19920512	US 1990-587791	19900925
SK 279658	B6	19990211	SK 1991-3130	19911015
HR 921250	B1	20000630	HR 1992-921250	19921112
US 5283352	A	19940201	US 1992-987245	19921207
LV 10236	B	19950620	LV 1993-805	19930630
LT 3770	B	19960325	LT 1993-915	19930831
US 5446194	A	19950829	US 1993-121617	19930916

PRIORITY APPLN. INFO.:

FI 1986-4875	A	19861128
GB 1987-12437	A	19870528
US 1987-126911	A3	19871127
YU 1989-21	A6	19890106
US 1990-587791	A3	19900925
US 1991-792655	B1	19911115
US 1992-987245	A3	19921207

OTHER SOURCE(S): MARPAT 109:128570

GI



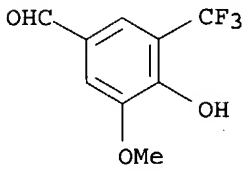
I

AB Title compds. I [R1,R2 = H, alkyl, (substituted) acyl, aroyl etc.; R1R2 = (cyclo)alkylidene; X = electroneg. substituent; R3 = H, halo, (substituted) alkyl, alkoxy, alkenyl, NO2, amino, amido etc.] are prepared for treating Parkinsonism. Condensation of 5.0 g 3,4-dihydroxy-5-nitrobenzaldehyde and 2.0 g cyclopentanone gave 78% 2,5-bis(3,4-dihydroxy-5-nitrobenzylidene)cyclopentanone which had IC50 of 3 nM as catechol-O-methyltransferase inhibitor in vitro.

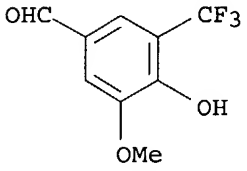
IT **116314-60-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiparkinson drug)

RN 116314-60-4 CAPLUS

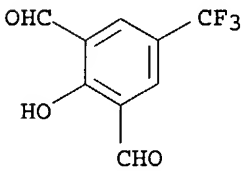
CN Benzaldehyde, 4-hydroxy-3-methoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **116314-60-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of antiparkinson pyrocatechol derivs.)
RN 116314-60-4 CAPLUS
CN Benzaldehyde, 4-hydroxy-3-methoxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:197158 CAPLUS
DOCUMENT NUMBER: 108:197158
TITLE: Role of the trifluoromethyl attractive group on the electrochemical and magnetic properties of copper(II) dinuclear compounds with Robson-type binucleating ligands
AUTHOR(S): Lacroix, Pascal; Kahn, Olivier; Theobald, Francois; Leroy, Jacques; Wakselman, Claude
CORPORATE SOURCE: Lab. Spectrochim. Elem. Transition, Univ.Paris-Sud, Orsay, 91405, Fr.
SOURCE: Inorganica Chimica Acta (1988), 142(1), 129-34
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB I·xH2O (X = CF3; m = 3, 4) were prepared I (X = CF3; m = 3) crystallizes in the orthorhombic system, space group Pbca, a 9.5737(4), b 18.072(10), c 34.340(11) Å, Z = 8. The structure consists of the expected Cu(II) dinuclear entities, with the ClO4- groups making addnl. bridges of either side of the macrocycle. The mol. skeleton is significantly bent in a boat fashion. The electrochem. properties of those 2 4-CF3-substituted compds. were studied and compared to those of the 4-Me analogs. The replacement of Me by CF3 shifts the 1st reduction wave by .apprx.0.15 V and the 2nd 1 by .apprx.0.18 V. The magnetic properties of I (X = Me, CF3) were compared. In spite of the modification of the redox properties, the singlet-triplet energy gaps J are equal within the exptl. uncertainties (J = -710(10) cm-1).
IT **114315-20-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with diaminopropane or diaminobutane in presence of cupric perchlorate)
RN 114315-20-7 CAPLUS
CN 1,3-Benzenedicarboxaldehyde, 2-hydroxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

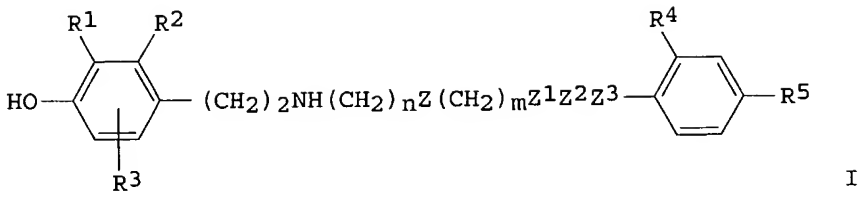


L22 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:5631 CAPLUS
DOCUMENT NUMBER: 104:5631
TITLE: Phenylethylamines and compositions containing them
INVENTOR(S): Dixon, John; Ince, Francis; Tinker, Alan Charles
PATENT ASSIGNEE(S): Fisons PLC, UK
SOURCE: Eur. Pat. Appl., 120 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 142283	A2	19850522	EP 1984-307102	19841017
EP 142283	A3	19860604		
EP 142283	B1	19910130		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
EP 375668	A2	19900627	EP 1990-200019	19841017
EP 375668	A3	19901017		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 60573	E	19910215	AT 1984-307102	19841017
US 4657929	A	19870414	US 1984-662348	19841018
US 4720586	A	19880119	US 1984-662393	19841018
CA 1258459	A1	19890815	CA 1984-465937	19841019
ZA 8408247	A	19850828	ZA 1984-8247	19841022
AU 8434594	A1	19850509	AU 1984-34594	19841023
AU 581415	B2	19890223		
NO 8404243	A	19850426	NO 1984-4243	19841024
NO 158460	B	19880606		
NO 158460	C	19880914		
FI 8404170	A	19850426	FI 1984-4170	19841024
DK 8405070	A	19850426	DK 1984-5070	19841024
JP 60115553	A2	19850622	JP 1984-222336	19841024
ES 537029	A1	19860616	ES 1984-537029	19841024
IL 73322	A1	19890131	IL 1984-73322	19841025
US 4791216	A	19881213	US 1986-938249	19861205
US 4803225	A	19890207	US 1987-127366	19871202
US 4885313	A	19891205	US 1987-127365	19871202
US 4868306	A	19890919	US 1988-260529	19881021

PRIORITY APPLN. INFO.:	
GB 1983-28489	19831025
GB 1983-28490	19831025
GB 1983-32447	19831206
GB 1983-32448	19831206
GB 1983-32452	19831206
GB 1984-1746	19840124
GB 1984-1747	19840124
GB 1984-1748	19840124
GB 1984-1750	19840124
EP 1984-307102	19841017
US 1984-662348	19841018
US 1984-662393	19841018
US 1986-938249	19861205

GI



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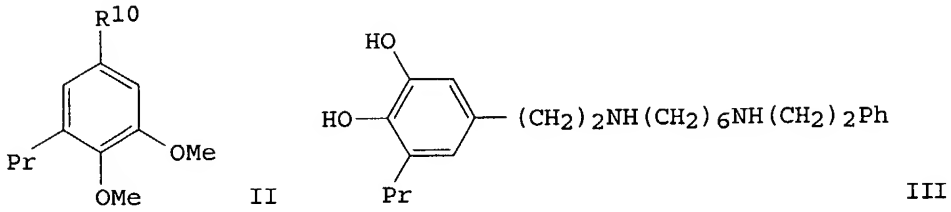


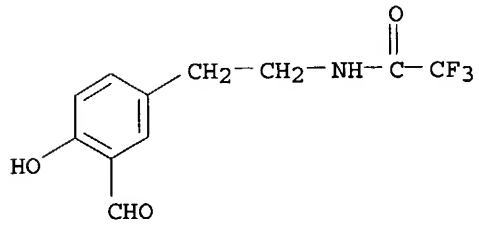
II III

AB Hydroxyphenethylamine derivs. I [R1 = OH, F, CH2R6, (un)substituted NH2; R2, R3 = H, F, Cl, Br, alkyl, NO2, cyano, (CH2)xR7, SR7; R1R2 = N:CHCH:CH, N:C(OH)CH:CH, NHCOCH2, o-NHC6H4; R4 = H; R5 = H, Cl; R6 = H, OH, alkyl, alkylsulfonyl; R7 = Ph, C6H4OH; Z = bond, C6H4, CH:CH, 1,4-cyclohexanediyl; Z1 = NH, O, S, SO2, CO, CH2, CONH, CO2; Z2 = (CH2)y, CO, CS, SO2, CH2CO, CHR8CH2, (R8R4 = CH2) CH2CH2 (un)substituted by 1-4 alkyls; Z3 = NR9 (R9 = H, alkyl), CH2, O, CO, S, SO2, bond; n, m = 1-4; x = 0-3; y = 1-3] were prepared Thus, aldehyde II (R10 = CHO) was reduced by NaBH4 to give II (R10 = CH2OH), which was treated with SOCl2 to give II (R10 = CH2Cl). Cyanation of the chloride by NaCN in Me2SO gave II (R10 = CH2CN), which was reduced by BH3-THF to II (R10 = CH2CH2NH2). Condensation of the amine with PhCH2CH2NHCO(CH2)4CO2H using N,N'-carbonyldiimidazole in CH2Cl2 gave II [R10 = (CH2)2NHCO(CH2)4CONH(CH2)2Ph], which was reduced by BH3-THF to II [R10 = (CH2)2NH(CH2)6NH(CH2)2Ph]. Cleavage of the di-Me ether by 48% aqueous HBr containing H3PO2 gave the diamine III. I act on peripheral and/or central dopamine receptors, thereby lowering blood pressure, reducing heart rate, and increasing renal blood flow. Some I exhibit cardiostimulant and bronchodilator effects (no data).

IT **99415-38-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and borohydride reduction of)

RN 99415-38-0 CAPLUS

CN Acetamide, 2,2,2-trifluoro-N-[2-(3-formyl-4-hydroxyphenyl)ethyl]- (9CI) (CA INDEX NAME)



L22 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:53828 CAPLUS
DOCUMENT NUMBER: 102:53828
TITLE: Improvement of lightfastness of dye images

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59083162	A2	19840514	JP 1982-193079	19821102

PRIORITY APPLN. INFO.: JP 1982-193079 19821102

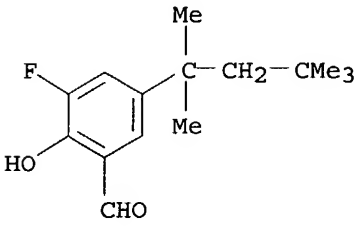
GI For diagram(s), see printed CA Issue.

AB The lightfastness of images formed from anilino type magenta coupler is improved by addition of I [M = Cu, Co, Ni, Pd, Pt; R = a H bonding group; R1-R3 = H, halo, OH, CN, alkyl, aryl, cycloalkyl, heterocyclyl; RR1, R1R2, or R2R3 together may form a 6-membered ring; R4 = H, alkyl, aryl] and ≥1 compound selected from II, III, IV, and V [R5 = H, alkyl, acyl, sulfonyl, carbamoyl, sulfamoyl, alkoxycarbonyl, trialkylsilyl; R6-R8 = H, alkyl, alkoxy, aralkyl, aryl, aryloxy, aralkoxy, alkenyl, alkenyloxy, acylamino, halo, alkoxycarbonyl, acyloxy, acyl, sulfonamido; R9 = C1-12 alkyl, alkoxy, arylthio, arylsulfinyl, arylsulfonyl, aralkyl, halo, aryl, acyl; R10 = H, C1-22 alkyl, alkoxy (different from R5O), aralkoxy (different of R5O), C1-22 alkylthio, aralkylthio, C2-22 acylamino, C2-22 acyl, C1-38 alkylamino, C6-32 arylamino, heterocyclic amino; R11 = H, halo, C1-22 alkyl, C6-22 arylthio, C1-22 alkylthio, C6-22 arylsulfonyl, C6-22 arylsulfinyl, C7-32 aralkyl, C6-32 aryl, C6-32 aryldithio, C6-32 aryloxy; R12 = H, C1-22 alkyl, C3-22 alkenyl; R13 = C1-22 alkyl, C3-22 alkenyl; R14 = alkyl, alkenyl, heterocyclyl, COR18, SO2R19, CONHR20; R15, R16 = H, halo, alkyl, alkenyl, alkoxy, alkenyloxy; R17 = H, alkyl, alkenyl, aryl; R18-R21 = alkyl, alkenyl, aryl, heterocyclyl; A = 5- or 6-membered ring, spiro rings] in the magenta dye image-retaining layer. Thus, VI, I (M = Ni; R = 2-ethylhexyloxy; R1-R4 = H), and VII were added to a green-sensitive Ag(Br,Cl) emulsion and the emulsion was used to prepare a photog. paper. The photog. paper was then imagewise exposed and developed to give a magenta image which showed excellent lightfastness.

IT **93968-52-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nickel acetate and hydroxylamine hydrochloride)

RN 93968-52-6 CAPLUS

CN Benzaldehyde, 3-fluoro-2-hydroxy-5-(1,1,3,3-tetramethylbutyl)- (9CI) (CA INDEX NAME)

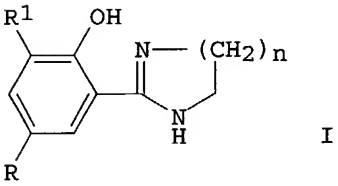


L22 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:505246 CAPLUS
DOCUMENT NUMBER: 99:105246
TITLE: Di-ortho-substituted phenols of which one of the substitutions is a heterocycle, antihypertensive medicines containing them and synthesis intermediates
INVENTOR(S): Teulon, Jean Marie
PATENT ASSIGNEE(S): CARPIBEM (Centre d'Activite et de Recherche

Pharmaceutique Industrielle Biologique et Medicale), Fr.
SOURCE: Eur. Pat. Appl., 60 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 70779	A2	19830126	EP 1982-401339	19820719
EP 70779	A3	19830622		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FR 2509730	A1	19830121	FR 1981-14011	19810717
FR 2509730	B1	19840106		
WO 8300333	A1	19830203	WO 1982-FR120	19820719
W: AU, BR, DK, FI, HU, JP, KP, MC, MG, MW, NO, RO, SU, US				
RW: CF, CG, CM, GA, SN, TD, TG				
AU 8287316	A1	19830317	AU 1982-87316	19820719
JP 58501127	T2	19830714	JP 1982-502218	19820719
ZA 8209273	A	19830928	ZA 1982-9273	19821217
DK 8301197	A	19830315	DK 1983-1197	19830315
PRIORITY APPLN. INFO.:			FR 1981-14011	19810717
			WO 1982-FR120	19820719

GI



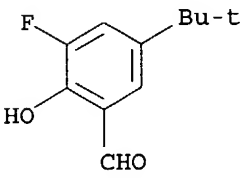
I

AB The phenols I (R = H, alkyl, cycloalkyl, alkoxy, alkylthio, halo; R1 = halo, NO2, OMe, SMe, SOMe, SO2Me, NHAc, allyl; n = 1-3) were prepared Thus, 2,4-ClCH2(Me3C)C6H3OMe was treated with Me2CHNO2 to give 2,5-MeO(Me3C)C6H3CHO which was converted to its oxime and dehydrated to give 2,5-MeO(Me3C)C6H3CN. Aminolysis of the latter compound with H2NCH2CH2NH2 gave I (R = CMe3, R1 = H, n = 1) which was treated with Br2 to give I.HBr (R = CMe3, R1 = Br, n = 1) (II). At 16 mg/kg orally in rats II gave a decrease in blood pressure of 69 mm 1 h after administration.

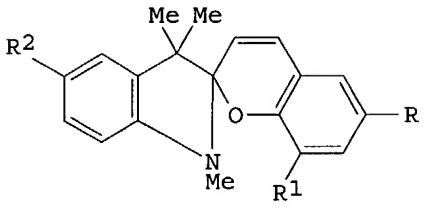
IT **85943-59-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, oximation, and dehydration of)

RN 85943-59-5 CAPLUS

CN Benzaldehyde, 5-(1,1-dimethylethyl)-3-fluoro-2-hydroxy- (9CI) (CA INDEX NAME)



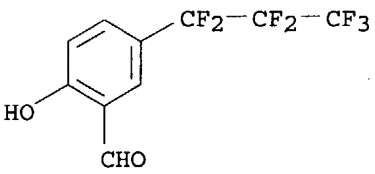
L22 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:499309 CAPLUS
DOCUMENT NUMBER: 95:99309
TITLE: Synthesis and photochromic properties of perfluoroalkyl and trifluoromethylsulfonyl substituted indoline spirochromenes
AUTHOR(S): Yagupol'skii, L. M.; Pasenok, S. V.; Gal'bershtam, M. A.; Bobyleva, G. K.; Popov, V. I.; Kondratenko, N. V.
CORPORATE SOURCE: Inst. Org. Chem., Kiev, 252660, USSR
SOURCE: Dyes and Pigments (1981), 2(3), 205-13
CODEN: DYPIDX; ISSN: 0143-7208
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A number of new perfluoroalkyl- and trifluoromethylsulfonyl-substituted indoline spirochromenes (I; R = C3F7, CF3SO2, NO2; R1 = H, NO2; R2 = H, CF3) were synthesized. The introduction of CF3SO2 or C3F7 groups into the chromene moiety of the I mol. resulted in their ability to undergo photochromic conversions. The dyes were examined by spectrophotometry and the rate consts. were determined for the fading reaction. Some correlations of the rate consts. with the electron withdrawing properties of the substituents were observed

IT **78914-93-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with Fischer's base and derivs.)
RN 78914-93-9 CAPLUS
CN Benzaldehyde, 5-(heptafluoropropyl)-2-hydroxy- (9CI) (CA INDEX NAME)



L22 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:150392 CAPLUS
DOCUMENT NUMBER: 84:150392
TITLE: Phenyl carbamates
INVENTOR(S): Nikles, Erwin; Dittrich, Volker; Pinter, Ladislaus
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: U.S., 7 pp. Division of U.S. 3,856,816.
CODEN: USXXAM
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3933858	A	19760120	US 1974-513607	19741010
JP 49008850	B4	19740228	JP 1965-61577	19651008
US 3781301	A	19731225	US 1971-197474	19711110
US 3856968	A	19741224	US 1971-199008	19711115
JP 51021976	B4	19760706	JP 1972-57376	19720610
US 3856816	A	19741224	US 1973-402650	19731001
US 3944674	A	19760316	US 1974-511408	19741002

PRIORITY APPLN. INFO.:

CH 1964-13113 A 19641008
US 1965-493256 A3 19651005
US 1968-782335 A2 19680513
US 1970-2445 A1 19700112
US 1971-197474 A3 19711110
US 1973-402650 A3 19731001
CH 1965-10789 A 19650730
US 1967-647274 19670428
US 1968-728335 A2 19680513
US 1968-728835 A2 19680513
US 1968-758616 A1 19680909
US 1971-199008 A3 19711115

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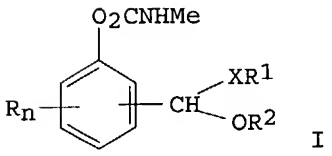
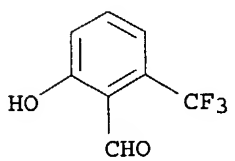


I

AB About 25 phenyl carbamates I [Rn = H, Me, F3C, Br2, (NO2)2, etc., R1 = R2 = Et or (R1R2) = alkylene; X = O, S], useful as insecticides, acaricides, herbicides, bactericides, fungicides, and molluscicides (insecticidal and acaricidal activity given), were prepared by converting m-hydroxybenzaldehyde or salicylaldehydes to their acetals and treating these with MeNCO. Thus, reaction of salicylaldehyde with ethylene glycol in C6H6 at elevated temperature in the presence of ZnCl2 and H3PO4 gave o-(1,3-dioxolan-2-yl)phenol, which was treated with MeNCO in PhMe in the presence of Et3N to give o-(1,3-dioxolan-2-yl)phenyl N-methylcarbamate. Among .apprx.10 more glycols used for acetalization of the aldehydes were 1,2-propanediol, 2,3-butanediol, glycerol, neopentyl glycol, and HSCH2CH2OH.

IT **58914-35-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with propanediol)

RN 58914-35-5 CAPLUS
CN Benzaldehyde, 2-hydroxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1951:52811 CAPLUS
DOCUMENT NUMBER: 45:52811
ORIGINAL REFERENCE NO.: 45:9001b-i,9002a-c
TITLE: Organic fluoro compounds. IV. The Hoesch reaction with trifluoromethyl and trichloromethyl cyanides
AUTHOR(S): Whalley, W. B.
CORPORATE SOURCE: Univ. Liverpool, UK
SOURCE: Journal of the Chemical Society, Abstracts (1951) 665-71
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 45:52811

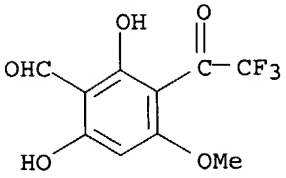
AB cf. C.A. 45, 3347e. m-C6H4(OH)2 (4 g.) in 125 mL. ether containing 3 g. ZnCl2, saturated at about -5° with HCl, treated with 12 g. F3CCN (prepared from F3CCONH2 and P2O5), kept 24 h. at 0°, and the product in 40 mL. H2O heated 15 min. on the steam bath, gives 4.7 g. α,α,α-trifluororesacetophenone (I), m. 103°. I (1 g.), 5 mL. MeI, 4 g. K2CO3, and 75 mL. Me2CO, refluxed 5 h., give 1 g. of the di-Me ether, m. 52°; when heated 15 min. on the steam bath with 15% KOH it yields CHF3 and 2,4-(MeO)2C6H3CO2H. 2,1,3-EtC6H3(OH)2 (2 g.) in 100 mL. ether containing 2 g. ZnCl2, saturated at 0° with HCl, treated with 7 g. F3CCN, kept 24 h. at 0°, and the product heated 15 min. on the steam bath with 40 cc. H2O, gives 2.5 g. 3-ethyl-α,α,α-trifluoro-2,4-dihydroxyacetophenone (II), m. 139°, strong red-brown color with alc. FeCl3. II with MeI and K2CO3 in Me2CO gives the di-Me ether (an oil) which on hydrolysis (15 min.) with 15% KOH gives 3,2,4-Et(MeO)2C6H2CO2H. 4,1,3-EtC6H3(OH)2 (2 g.) yields 2.4 g. of the 5-Et isomer of II, m. 99°; di-Me ether, m. 65°. 5,1,3-MeOC6H3(OH)2 (4 g.) and 12 g. F3CCN give 2.2 g. α,α,α-trifluoro-2,4-dihydroxy-6-methoxyacetophenone (III), pale yellow, m. 154°, strong red-brown color with alc. FeCl3. III (1 g.) in 75 mL. ether containing 0.5 g. Zn(CN)2 and 4 mL. HCN, saturated at 0° with HCl, kept 24 h., and hydrolyzed with H2O (24 min. on the steam bath), gives 0.3 g. of the 3-formyl derivative, m. 129°, red-brown color with alc. FeCl3 [2,4-dinitrophenylhydrazone, orange-yellow, m. 278° (decomposition)]; the CF3 group could not be removed by alkaline hydrolysis. III with Me2SO4 and K2CO3 gives a quant. yield of α,α,α-trifluoro-2,4,6-trimethoxyacetophenone, m. 60°, which also results (1.7 g.) from 1 g. C6H3(OMe)3 and F3CCN. 4,1,3-HOC6H3(OMe)2 (3 g.) yields 3 g. α,α,α-trifluoro-2-hydroxy-4,5-dimethoxyacetophenone, pale yellow-green, m. 82°, olive-green color with alc. FeCl3. 6-Methoxy-3-methylcoumarone (2 g.) gives 3 g. of the 2-trifluoroacetyl derivative, very pale yellow, m. 87°; hydrolysis with 2 N NaOH gives 100% of the 2-carboxylic acid. 1,3,5-C6H3(OH)3, 1,2,3-C6H3(OH)3, and 5,1,3-MeC6H3(OH)2 do not react with F3CCN. The α,α,α-trifluoroacetophenones do not yield 2,4-dinitrophenylhydrazones and are rather surprisingly stable to the action of alkali but under moderately vigorous conditions undergo fission to give a gas (CHF3) and the corresponding acid, usually in small yield because of partial decarboxylation. Attempted Clemmensen reduction causes rapid resinification. The compds. are easily soluble in NaHCO3. Cl3CCN does not react with m-C6H4(OH)2, 1,3,5-C6H3(OH)3, 1,2,3-C6H3(OH)3, and 5,1,3-MeC6H3(OH)2. 5,1,3-MeOC6H3(OH)2 (5 g.) and 10 g. Cl3CCN with HCl at 0° give 4-5 g. α,α,α-trichloro-2,4-dihydroxy-6-methoxyacetophenone (V), pale cream, m. 152°, weak red-brown color with FeCl3. 6,2,4-MeO(HO)C6H3Ac (1 g.) in 20 mL. MeOH, added to 10 g. Zn-Hg, 20 mL. concentrated HCl, and 10 mL. H2O and refluxed 4 h., gives 0.6 g. 1-ethyl-2,4-dihydroxy-6-methoxybenzene (VI), m. 109° [bis(p-nitrobenzoate), pale cream, m. 164°]; similar reduction of 0.9

g. V gives 0.3 g. VI. VI (2 g.) in 12 mL. 2 N NaOH, acidified after 30 min. with 2 N HCl, gives 1.1 g. 2,4-dihydroxy-6-methoxybenzoic acid, m. 200° (decomposition), deep red-brown color with alc. FeC3; Me ester (VII), m. 194°, deep red-brown color with alc. FeCl3. V (0.5 g.) in 10 mL. MeOH containing 1 drop 60% KOH, refluxed 5 min., gives 0.35 g. VII. VII (0.8 g.) in 150 mL. ether containing 0.5 g. Zn(CN)2 and 5 mL. HCN, saturated at 5° with HCl, kept 24 h., and hydrolyzed with H2O, gives 0.7 g. of the 3-formyl derivative (VIII), m. 184°, deep red-brown color with alc. FeCl3 [2,4-dinitrophenylhydrazone, brick-red, m. 294° (decomposition)]. VIII (0.5 g.) and 5 mL. 2 N NaOH, refluxed 45 min. in a N atmospheric, give a small quantity of 4,2,6-MeO(HO)2C6H2CHO. V (1.5 g.) in 100 mL. ether containing 1 g. Zn(CN)2 and 5 mL. HCN, saturated at 0° with HCl and the product hydrolyzed, gives 1.2 g. of the 3-formyl derivative (IX), m. 150°, red-brown color with alc. FeCl3 [2,4-dinitrophenylhydrazone, bright crimson, m. 247° (decomposition)]; hydrolysis with 2 N NaHCO3 gives about 100% 2,4-dihydroxy-3-formyl-6-methoxybenzoic acid, m. 185° (decomposition), deep red-brown color in alc. FeCl3; boiled with H2O containing a little MeOH, it gives 4,2,6-MeO(HO)2C6H2CHO, m. 141-2°. Reduction of 0.5 g. IX in 10 mL. MeOH by refluxing 10 min. with 10 mL. concentrated HCl, 5 mL. H2O, and 5 g. amalgamated Zn gives 0.3 g. 3-ethyl-2,6-dihydroxy-4-methoxytoluene, m. 112° [bis(p-nitrobenzoate), very pale greenish yellow, m. 178°]. 1,3,5-C6H3(OMe)3 (5 g.) and 10 g. Cl3CCN give 3.5 g. α,α,α-trichloro-2,4,6-trimethoxyacetophenone, m. 116°; reduction gives a nearly quant. yield of 2,4,6-(MeO)3C6H2Et, m. 28°. m-HOC6H4OMe (2 g.) and 4 g. Cl3CCN give 1.5 g. α,α,α-trichloro-4-hydroxy-2-methoxyacetophenone, m. 144°; in cold 2 N NaHCO3 it gives 2,4-MeO(HO)C6H3CO2H. 4,1,2-HOC6H3(OMe)2 (2 g.) and 4 g. Cl3CCN give 1 g. α,α,α-trichloro-2-hydroxy-4,5-dimethoxyacetophenone, yellow, m. 107°, green-brown color with alc. FeCl3; cold 2 N NaOH gives a quant. yield of 2,4,5-HO(MeO)2C6H2CO2H. 6-Hydroxy-3-methylcoumarone (0.5 g.) gives 0.3 g. of the 2-trichloroacetyl derivative, pale greenish yellow, m. 180°; with MeI and K2CO3 in boiling Me2CO, it gives a quant. yield of Me 6-methoxy-3-methylcoumarone-2-carboxylate, m. 90°. 6-Methoxy-3-methylcoumarone gives the 2-trichloroacetyl derivative, pale yellow, m. 154°; 2 N NaOH gives CHCl3 and the 2-carboxylic acid, m. 190°.

IT **10116-93-5**, γ-Resorcylaldehyde, 4-methoxy-3-trifluoroacetyl- (preparation of)

RN 10116-93-5 CAPLUS

CN γ-Resorcylaldehyde, 4-methoxy-3-(trifluoroacetyl)- (8CI) (CA INDEX NAME)



L22 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1950:19933 CAPLUS

DOCUMENT NUMBER: 44:19933

ORIGINAL REFERENCE NO.: 44:3919e-i,3920a-e

TITLE: Organic fluoro compounds. I. Hydroxy derivatives of benzotrifluoride

AUTHOR(S): Whalley, W. B.

CORPORATE SOURCE: Univ. of Liverpool, UK

SOURCE: Journal of the Chemical Society, Abstracts (1949) 3016-20
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

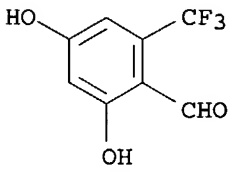
AB 3,5-O2N(H2N)C6H3CF3 (I) (C.A. 39, 505.1) (5 g.) in 17 mL. H2O and 20 mL. concentrated H2SO4 at 0°, diazotized with 1.9 g. NaNO2 in 10 mL. H2O and (after 15 min.) added to 250 cc. boiling saturated aqueous CuSO4, gives 2.5 g. 3-nitro-5-hydroxybenzotrifluoride (II), pale yellow, m. 92° (decreased yield with larger quantities of I). II (10 g.) in 50 mL. boiling EtOH, gradually treated with 50 g. Na2S in 200 mL. EtOH, refluxed 1.5 h., treated with 25 mL. 10% EtOH-NaOH, refluxed an addnl. hr., acidified with HCl, and neutralized with NaHCO3, gives 8 g. 3-amino-5-hydroxybenzotrifluoride (III), pale buff, m. 81° (di-Ac derivative, m. 138°). Through the diazo reaction, 5 g. III yields 2.5 g. 3,5-dihydroxybenzotrifluoride (IV), with 1 mol. H2O, b0.001 120°, m. 54° (anhydrous, m. 65°), deep violet FeCl3 reaction; bis(p-nitrobenzoate), m. 166°; bis(phenylazo) derivative, bright crimson, m. 233-4° (decomposition). 3,5-(O2N)2C6H3CF3 (5 g.), reduced (20 min.) in 100 mL. EtOH over Pd-C, yields 3.5 g. 3,5-diaminobenzotrifluoride, m. 88°, slowly oxidized in solid state or in solution; di-Ac derivative, m. 298°. IV (1 g.), 1 g. Zn(CN)2, 2 mL. HCN, and 25 mL. C6H6 at 0°, treated slowly with 1 g. AlCl3 and then (4 h.) with HCl, and the C6H6 solution decomposed with dilute HCl and ice and distilled with steam, give 0.1 g. 3,5-dihydroxy-2-formylbenzotrifluoride, m. 147°, reddish-brown FeCl3 reaction [2,4-dinitrophenylhydrazone, bright scarlet, m. 276° (decomposition)]. I (5 g.) in 15 mL. concentrated HCl and 15 mL. H2O, diazotized as above, yields 3 g. 3,5-Cl(O2N)C6H3CF3, pale yellow, b760 206-8°, characterized by reduction (Sn and HCl) and acetylation to 3-chloro-5-acetamidobenzotrifluoride (V), m. 134°. V (3 g.) was prepared also by the addition of the diazonium chloride from 5 g. I to CuCl in 1:1 HCl, reduction, and acetylation. 2,5-O2N(HO)C6H3CF3 (VI) (3.6 g.), reduced with alc. Na2S, gives 1.4 g. 2-amino-5-hydroxybenzotrifluoride (VII), m. 158°; reduction of 10 g. VI with 10 g. Sn and 25 mL. concentrated HCl gives 6 g. VII; di-Ac derivative, m. 142°. Through the diazo reaction in H2SO4, 5 g. VII yields 1 g. 2,5-dihydroxybenzotrifluoride (VIII), m. 109°; VIII results in 3.5-g. yield by adding (4 h.) 16.5 g. K2S2O8 (saturated aqueous solution) to 10 g. m-HOC6H4CF3 in 140 mL. 2 N NaOH at 0° and allowing the mixture to stand 24 h.; VIII gives an olive-green FeCl3 reaction; bis(p-nitrobenzoate), m. 230°; 0.3 g. VIII in 2 N NaOH (3 h.) gives 0.3 g. 2,5-(HO)2C6H3CO2H. 2,5-O2N(H2N)C6H3CF3 (10 g.) in 30 mL. concentrated HCl and 20 mL. H2O at 0°, diazotized and poured into 400 mL. boiling saturated aqueous CuSO4, gives 6.4 g. 5-chloro-2-nitrobenzotrifluoride, pale yellow, b760 224°; reduction of 4 g. and acetylation give 4 g. 5-chloro-2-acetamidobenzotrifluoride, m. 148°. 3,4-H2N(MeO)C6H3CF3 (6 g.) yields 2.8 g. 3-hydroxy-4-methoxybenzotrifluoride (IX), b12 104-5°, characterized as the p-nitrobenzoate, m. 120°; 4 g. IX and 5 mL. HI (d. 1.7), refluxed 5 min., give 1.9 g. IX and 1 g. 3,4-HO(MeO)C6H3CO2H. IX (6 g.) and 6.5 g. KOH in 60 mL. H2O, treated (6 h.) with 8.5 g. K2S2O8, yield 2.8 g. IX and 0.5 g. 2,5-dihydroxy-4-methoxybenzotrifluoride, m. 136°; bis(p-nitrobenzoate), m. 227°; with cold 2 N NaOH, it yields 4,2,5-MeO(HO)2C6H2CO2H, characterized as asaronic acid. The diazo solution from 21 g. 3-H2NC6H4CF3 (X) in HCl, added to 400 mL. boiling saturated CuSO4, gives 15.7 g. 3-ClC6H4CF3 and 2 g. 3-HOC6H4CF3 (XI). PhN2Cl (6.5 g. PhNH2), added to 10 g. XI and 9 g. NaOH in 150 mL. H2O, gives 5 g. 2-phenylazo-5-hydroxybenzotrifluoride, reddish brown, m. 118° (decomposition); fission with Na2S2O4 in 50% EtOH gives VII. Attempts to mononitrate XI failed; under mild conditions no reaction occurred and more vigorous conditions gave rise to polynitrophenols. X (5 g.) in 50 mL. concentrated H2SO4 and 40 mL.

AcOH at 0°, treated with 5 mL. fuming HNO3 in 20 mL. concentrated H2SO4 and allowed to stand 4 days, give 7 g. of a 4,6-di-NO2 derivative (?), pale lemon-yellow, m. 126° (decomposition); acetate, golden yellow, m. 149° (decomposition).

IT **320-13-8**, o-Orsellinaldehyde, α,α,α-trifluoro-
(preparation of)

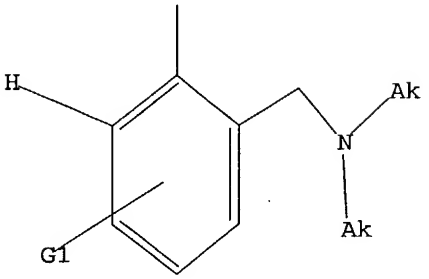
RN 320-13-8 CAPLUS

CN Benzaldehyde, 2,4-dihydroxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



=>

HAS NO ANSWERS
L7 STR



F

G1 MeO,EtO,n-BuO,CHO,C(O)CH3,O,S

Structure attributes must be viewed using STN Express query preparation.

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=> s l7
SAMPLE SEARCH INITIATED 13:02:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2343 TO ITERATE

 42.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        43957 TO    49763
PROJECTED ANSWERS:               0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 full
FULL SEARCH INITIATED 13:02:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  47580 TO ITERATE

100.0% PROCESSED   47580 ITERATIONS                              18 ANSWERS
SEARCH TIME: 00.00.01

L9            18 SEA SSS FUL L7

=>  dcan
DCAN IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d scan

L9   18 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl](2-
     pyridinylmethyl)amino]methyl]-4-hydroxyphenoxy]-3,5-
     dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF   C32 H32 F N3 O5
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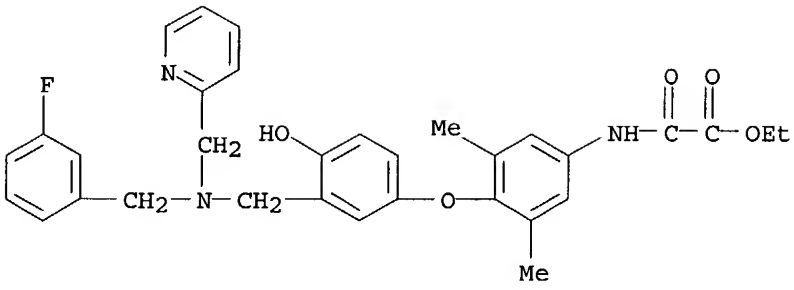
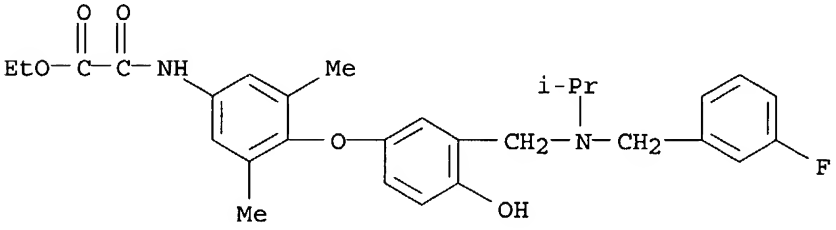


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

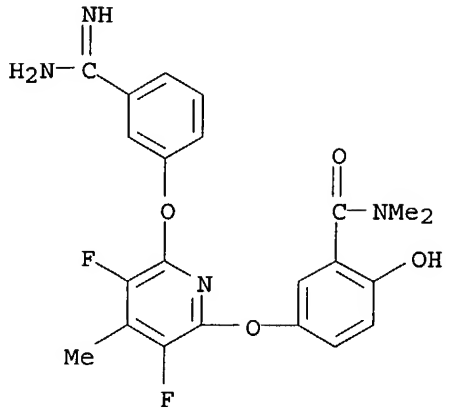
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl](1-methylethyl)amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C29 H33 F N2 O5



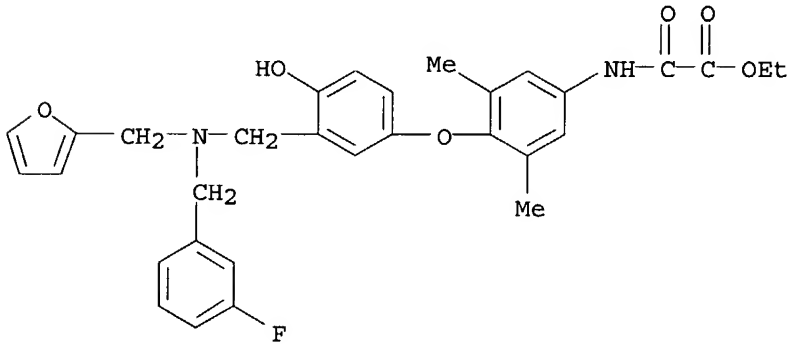
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzamide, 5-[[6-[3-(aminoiminomethyl)phenoxy]-3,5-difluoro-4-methyl-2-pyridinyl]oxy]-2-hydroxy-N,N-dimethyl- (9CI)
MF C22 H20 F2 N4 O4
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl](2-furanylmethyl)amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C31 H31 F N2 O6

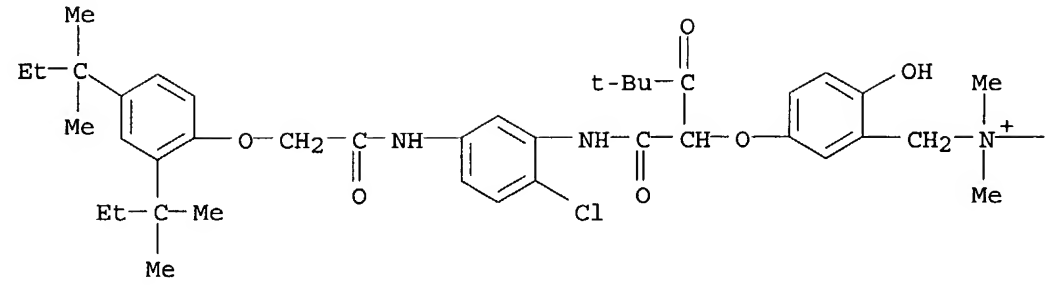


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

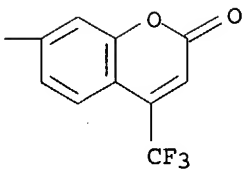
L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2H-1-Benzopyran-7-aminium, N-[[5-[1-[[[5-[[[2,4-bis(1,1-dimethylpropyl)phenoxy]acetyl]amino]-2-chlorophenyl]amino]carbonyl]-3,3-dimethyl-2-oxobutoxy]-2-hydroxyphenyl]methyl]-N,N-dimethyl-2-oxo-4-(trifluoromethyl)-, chloride (9CI)
MF C50 H58 Cl F3 N3 O8 . Cl

PAGE 1-A

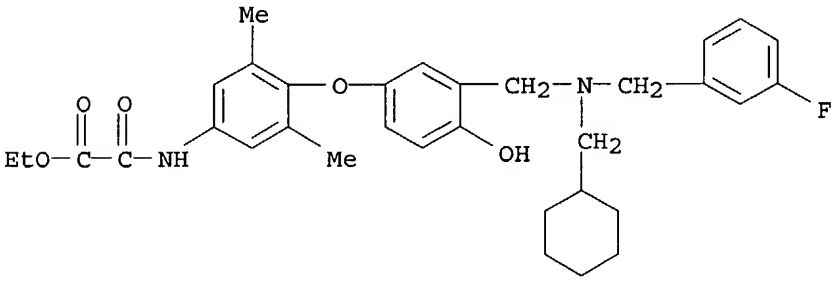


● Cl⁻

PAGE 1-B

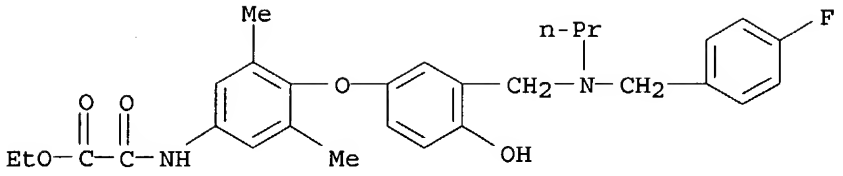


L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[(cyclohexylmethyl)[(3-fluorophenyl)methyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C33 H39 F N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(4-fluorophenyl)methyl]propylamino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C29 H33 F N2 O5

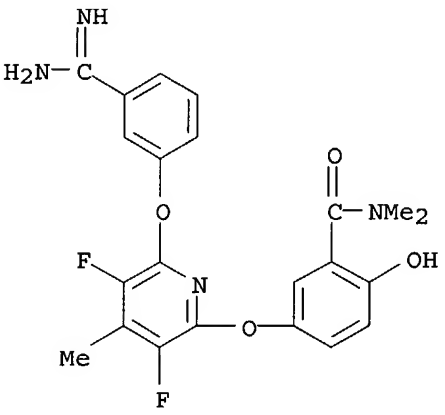


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

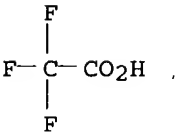
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzamide, 5-[[6-[3-(aminoiminomethyl)phenoxy]-3,5-difluoro-4-methyl-2-pyridinyl]oxy]-2-hydroxy-N,N-dimethyl-, trifluoroacetate (5:6) (salt) (9CI)
MF C22 H20 F2 N4 O4 . 6/5 C2 H F3 O2

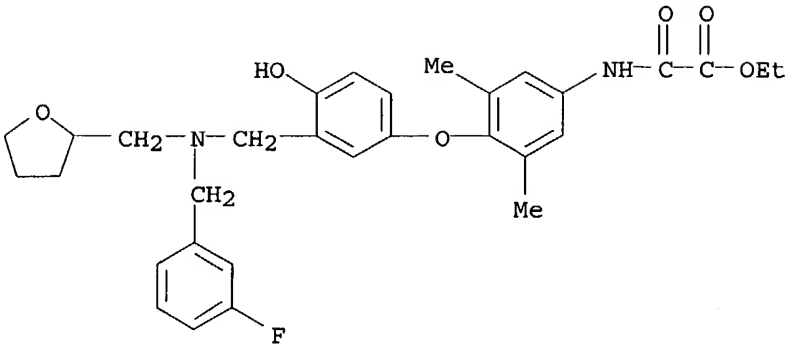
CM 1



CM 2



L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl][(tetrahydro-2-furanyl)methyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C31 H35 F N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Ethanone, 1-[3-[(dimethylamino)methyl]-2,4-dihydroxyphenyl]-2-(4-fluorophenoxy)- (9CI)
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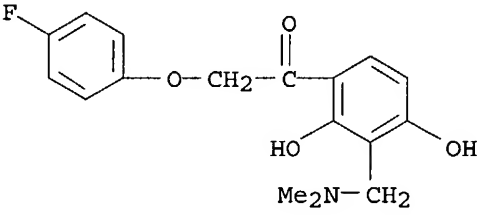

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl][2-(2-pyridinyl)ethyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
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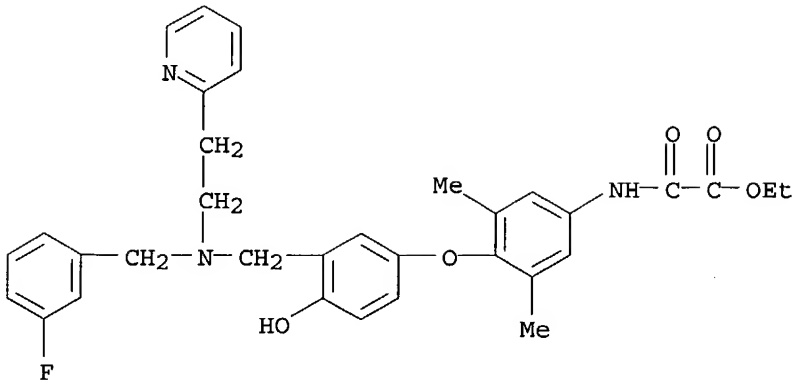
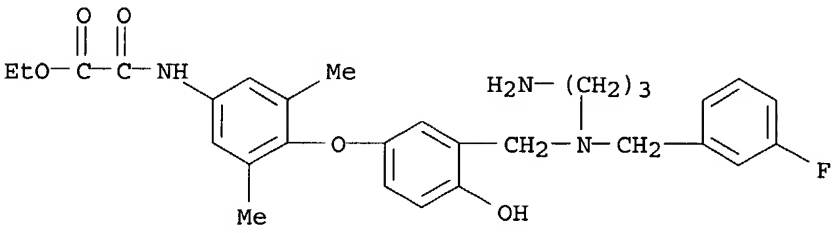


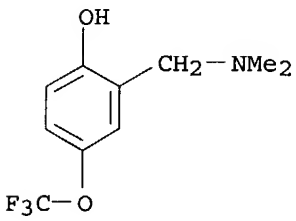
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[(3-aminopropyl)[(3-fluorophenyl)methyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C29 H34 F N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

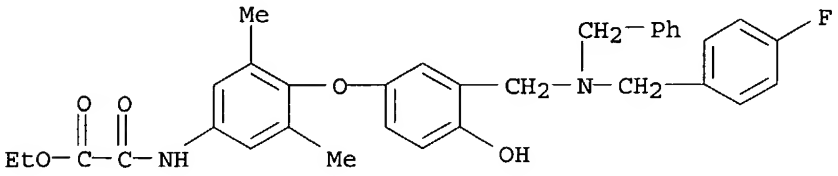
L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Phenol, 2-[(dimethylamino)methyl]-4-(trifluoromethoxy)- (9CI)
MF C10 H12 F3 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

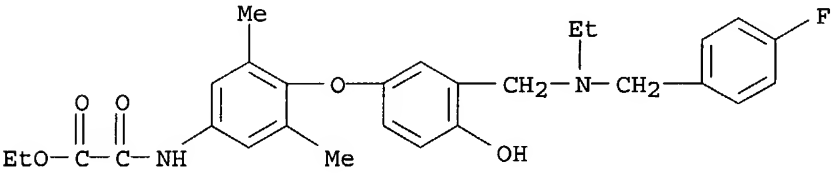
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(4-fluorophenyl)methyl](phenylmethyl)amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C33 H33 F N2 O5



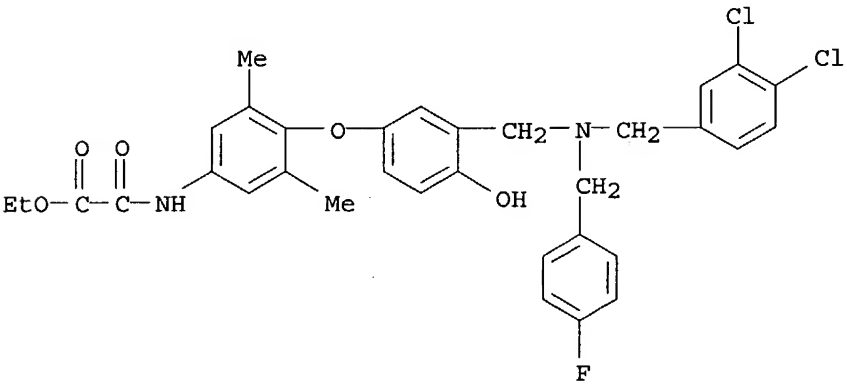
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[ethyl[(4-fluorophenyl)methyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C28 H31 F N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

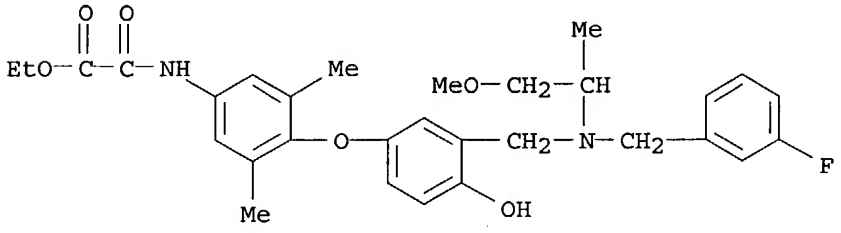
L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3,4-dichlorophenyl)methyl][(4-fluorophenyl)methyl]amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C33 H31 Cl2 F N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

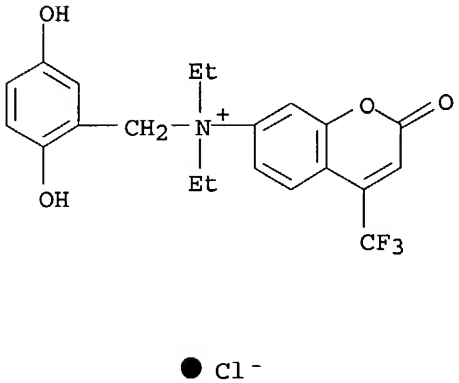
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetic acid, [[4-[3-[[[(3-fluorophenyl)methyl](2-methoxy-1-methylethyl)amino]methyl]-4-hydroxyphenoxy]-3,5-dimethylphenyl]amino]oxo-, ethyl ester (9CI)
MF C30 H35 F N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 18 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 2H-1-Benzopyran-7-aminium, N-[(2,5-dihydroxyphenyl)methyl]-N,N-diethyl-2-oxo-4-(trifluoromethyl)-, chloride (9CI)
MF C21 H21 F3 N O4 . Cl



ALL ANSWERS HAVE BEEN SCANNED